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Special Reports

INDIRECTLY FUNDED RESEARCH AND EXPLORATORY DEVELOPMENT AT THE APPLIED PHYSICS LABORATORY

FISCAL YEAR 1975

THE JOHNS HOPKINS UNIVERSITY ■ APPLIED PHYSICS LABORATORY

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RESEARCH AND EXPLORATORY DEVELOPMENT
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FISCAL YEAR 1975

R. W. HART, EDITOR

THE JOHNS HOPKINS UNIVERSITY ■ APPLIED PHYSICS LABORATORY
Johns Hopkins Road, Laurel, Maryland 20810
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THE JOHNS HOPKINS UNIVERSITY
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LAUREL, MARYLAND

ABSTRACT

This report summarizes the Indirectly Funded Research and Exploratory Development activities of the Applied Physics Laboratory during fiscal year 1975 (1 October 1974 - 30 September 1975).

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THE INDIRECTLY FUNDED RESEARCH AND EXPLORATORY DEVELOPMENT PROGRAM

The Applied Physics Laboratory is primarily engaged in Navy-funded engineering development tasks. These tasks have specific operational goals, require dedicated engineering effort to meet rigid time scales, and therefore use primarily state-of-the-art technology. Yet, innovation and advancement of the state of the art is essential to continued vitality. In recognition of the importance of basic and exploratory research for these purposes, the Laboratory conducts an Indirectly Funded Research and Exploratory Development Program through which a small fraction of its efforts is devoted to fundamental and exploratory research not explicitly provided for within the directly funded tasks.

The objectives of this program remain constant:

1. To provide current, in-depth understanding of technical fields of importance to the Laboratory's applied tasks;

2. To originate and explore new concepts of potential importance to the solution of national problems; and

3. To provide a window into science to cultivate the technical competence of the Laboratory, as an organization devoted to development and engineering tasks.

Whereas no one Laboratory may make a major contribution in a given field and a given year, it is necessary to be continually at the forefront of research in order to be aware and appreciative of new developments in basic science, wherever they occur, to grasp their significance for new technology, and to be able to convey the essence and applicability of these discoveries to the engineers who need this information to solve specific problems and enhance the capabilities of systems or components.

To achieve these objectives, the IR&D program is organized into two major components:

1. Research, carried out in the Research Center of the Laboratory, encompassing mainly long-term, scientifically based investigations looking toward the interdisciplinary transfer of advancing science into the Laboratory's technology, and

2. Exploratory Development, comprised of mainly short-term investigations, specifically authorized by the Director, emphasizing the evolution of technology through early stages of development of new ideas applicable to hardware systems, components, and materials.

The IR&D program has made and continues to make important contributions to science and technology in general and to the Navy and the Laboratory in particular. Foremost among these has been the concept of doppler navigation by Research Center scientists that led to the Navy Satellite Navigation System. Other notable developments described in previous reports of this series include detection and tracking of aircraft leading to the Navy AN/SYS-1 automated detection and tracking systems, dual-mode Redeye, the Box-Launcher, and Electrostatic Stabilization of Aircraft. The program also continues to make widely recognized contributions in areas such as chemical propulsion and laser technology. Projects in all of these and many other areas have been initiated by the IR&D program and subsequently supported by various DoD agencies.

With the encouragement of the Secretary of Defense and the Department of the Navy, the Laboratory also assumes a role in urgent nondefense problem areas. During the present fiscal year, about 15% of the Laboratory's efforts were devoted to projects directly funded by civilian agencies, including the National Aeronautics and Space Administration, the Federal Aviation Administration, the National Institutes of Health, the Energy Research and Development Administration, and the State of Maryland. Accordingly, whereas the major part of the program is defense oriented, it also uses IR&D funds derived from non-DoD sponsors to support investigations in primarily civilian areas.

These investigations have produced many important contributions, as described in previous reports of this series. Significant new developments continue to emerge, as described in subsequent sections of the present report, where the quality of the work is indicated by the cited recognition accorded many of the investigators.

THE RESEARCH CENTER

Introduction

The purpose of the Research Center is to contribute to the scientific and technological vitality of the Laboratory: to advance new concepts, to apply existing concepts in new areas, and to stimulate the transfer of advances from the forefront of science to technology. Results are published in the professional literature.

The IR&D program constitutes about two-thirds of the Research Center's efforts. It provides the long-term continuity essential to in-depth and up-to-date understanding and facility in fields of importance to the Laboratory's present and future technology. Research is conducted both independently and in collaboration with colleagues at universities and at industrial, government, and not-for-profit laboratories. Results are routinely presented at meetings of professional societies and published in the professional literature. More than 700 papers have been published in dozens of fields of physics, chemistry, mathematics, engineering, and life sciences. To disseminate information to other divisions of the Laboratory, the Research Center conducts seminars reporting on national and international scientific meetings and on its own research, and also contributes to ongoing tasks through consultations and/or direct funded participation.

The Research Center is comprised of a staff of 40 broadly trained senior professional investigators and 7 associate scientists (physicists, chemists, engineers, and mathematicians), who are assisted by a supporting staff of 15 technicians, machinists, and secretaries. Laboratory facilities for advanced research in fields of long-term and/or emerging significance include a mass spectrometry laboratory, a solid-state laboratory (with sputter-ion mass spectrometer), a spectroscopic laboratory (ultraviolet, optical, and infrared), a microwave physics laboratory, a molecular free-radical laboratory, a gas kinetic laboratory (with fast-flow reactor), and a scanning electron microscopy laboratory with ultra-high vacuum capability for surface studies.

Overview, 1975

Through the IR&D program, the Research Center continues to conduct broad scientific and technological research activities in selected areas which change with time in concert with the advancing needs of the Laboratory and new developments in science and technology. The present period has been productive. A total of 62 Research Center publications appeared in print, and 23 additional manuscripts were accepted for future publication. Nationally and internationally recognized stature has been maintained. During

the present fiscal year, Dr. K. Moorjani (Solid-State Physics Group) was visiting professor at the University of Grenoble; a national geophysical conference was dedicated to Dr. A. J. Zmuda (died July 1974) of the Electronics Physics Group; Dr. F. J. Adrian (Microwave Physics Group) was named Associate Editor of the Journal of Chemical Physics; and Dr. V. O'Brien (Theoretical Problems Group) was named to present one of three invited papers at the Biophysical Fluid Mechanics Symposium at the Spring Meeting of the American Physical Society. Numerous invitations were extended to participate in conferences and workshops, three with funding support from foreign agencies and two with funding support from national agencies.

The IR&D program continues as an orderly unfolding of the work of previous years, with research in seven general areas: (a) Applied Analysis, (b) Applied Mathematics, (c) Atomic, Molecular, and Electronic Physics, (d) Chemical Physics, (e) Microwave Physics, (f) Quantum Electronics and Excitation Mechanisms, and (g) Solid-State Physics. The nature of the projects and significant results are indicated in the subsequent sections of this report.

Technical Highlights

It is noteworthy that the present year marks certain particularly significant shifts of emphasis. First, the Research Center had long maintained a small (2 man-years) but distinguished space physics project carried on in the Electronics Physics Group by Dr. A. J. Zmuda and Dr. T. A. Potemra. The Research Center's ability to carry on such research effectively was severely compromised by the death of Dr. Zmuda in July 1974. Accordingly, with the beginning of the present fiscal year on 1 October 1974, Dr. Potemra and the project were transferred to the Space Development Department where work continues under the Exploratory Development phase of the IR&D program. Thus, for the first time in many years, the Research Center IR&D program has no space-physics component.

Second, there is a general trend in five of the above seven project areas away from concern with bulk phases and toward increased concern with interfacial and near-surface physics and chemistry. This reflects a widespread and accelerating surge of activity in the scientific community and an expectation that important new technology in electronics and energy-related areas will emerge. In general, surface and near-surface phenomena are difficult to study both theoretically and experimentally and are not thoroughly understood. Recent acquisition of a sputter-ion

mass spectrometer and the acquisition, this year, of an ultra-high-vacuum scanning electron microscope have facilitated increasing efforts in these areas.

Third, a particularly significant shift of emphasis has occurred within the Applied Mathematics Project. Much of the previous concern with the advancement of general methods is now applied to the specific area of stratified flow. Stratified flow, particularly phenomena associated with the movement of submerged bodies, is of great concern and is very incompletely understood. The present application of advanced mathematical techniques to such phenomena has already made significant contributions.

Finally, it is noteworthy that a project dealing with the properties of the internal and external electromagnetic fields of waveguides in the presence of anisotropic and absorptive media came to a close with the retirement of Dr. A. I. Mahan on 31 December 1974. Dr. Mahan has had a long and distinguished career, the last 19 years being at this Laboratory. He has been Treasurer of the Optical Society of America since 1960 and Associate Editor of the society's journal since 1961. Dr. Mahan continues to be associated with the Laboratory as a part-time assistant to the Chairman of the Research Center. During the past year, he was asked to present his work at international meetings in France and in Czechoslovakia for which the National Academy of Science appointed him alternate delegate to represent the Academy and the National Research Council.

APPLIED ANALYSIS

The Applied Analysis component of the IR&D program is directed toward maintenance and development of innovative capability in new theoretical techniques applicable to a broad spectrum of problem areas of importance to the Laboratory, the Navy, DoD, and the nation.

Emphasis continues to be placed in four general areas: theoretical chemistry, wave phenomena, statistical methods, and mechanics of fluids. The research is carried out through the part-time efforts of eight senior scientists and one associate scientist, in several instances with the collaboration of scientists in other divisions and at other institutions not funded by the APL IR&D program. Fifteen publications were issued during the present reporting period, and five others were accepted for future publication. Two of the APL scientists received invitations and financial support to participate in internationally sponsored workshops. Dr. M. H. Friedman, Supervisor of the group, continues to serve as (part-time) Associate Professor of Ophthalmology in The Johns Hopkins University School of Medicine. He is a Fellow of the American Institute of Chemists and a recipient of the National Capital Award of the District of Columbia Council of Engineering and Architectural Societies.

Theoretical Chemistry: Molecular Structure and Reactivity

Valence-bond theory has been exploited to predict the outcome of concerted chemical reactions, based on the molecular symmetry properties of the reacting molecules. Accurate determination of the electronic structure of several diatomic molecules has been accomplished by applying the diagrammatic techniques of many-body perturbation theory.

Chemical reactions lie at the heart of combustion, propulsion, and a vast number of energy-related phenomena of DoD and civilian importance. Assured capability to achieve new and improved reactions depends in large part on developing an improved quantitative understanding in fundamental, atomic/molecular terms. The studies in theoretical chemistry are a continuing effort to develop this capability.

The general method of approach is primarily through sophisticated techniques of many-body perturbation theory (MBPT), and has been carried out by Dr. D. M. Silver, of APL, and with collaborators at other institutions who are not funded by the IR&D program.

The work continues to be outstandingly successful as measured by published results and the wide recognition accorded them. During the present period, for example, Dr. Silver was invited to and attended the summer workshop on Collisions on Excited State Potential Energy Surfaces sponsored by the Centre Européen de Calcul Atomique at Moléculaire, expenses being paid by the French government. He also received, from the U.S. National Research Council, National Academy of Sciences, an award to attend the XXV International Congress of Pure and Applied Chemistry, Jerusalem, 6-11 July 1975. In addition, he was invited by The Johns Hopkins University Department of Chemistry to give a series of lectures on his research during the forthcoming academic year.

The development and understanding of selection rules is of wide importance to reaction chemistry and has constituted one phase of the program, as described in a previous report of this series. A new set of selection rules for concerted chemical reactions has been developed using the valence-bond theory to describe the structure of the molecules undergoing reaction; the methods are described in detail in a comprehensive publication (Ref. 1) in collaboration with Prof. M. Karplus of Harvard University. Using these methods, complicated molecular species can be analyzed in terms of pairs of electrons. The selection rules can then be applied to predict the feasibility of a reaction occurring. These predictive rules are of particular value in synthetic organic chemistry and in analyzing fast chemical reactions involved in combustion and upper atmospheric processes.

The properties of individual reaction paths at critical points on potential energy surfaces are of special importance in understanding the unfolding of reactions, and a mathematical examination of these (Ref. 2) was carried out in collaboration with E. A. McCullough of Utah State University. The study shows that a path of steepest descent follows a smooth kinkless trajectory. Such information is particularly relevant to studies of the dynamics of chemical reactions. Classical mechanical trajectory calculations on a bimolecular reaction (Ref. 3), carried out in collaboration with Dr. N. J. Brown of the University of California, Berkeley, are found to be quite sensitive to the detailed nature of the interaction potential. Hence, the most powerful methods (e.g., many-body perturbation theory) are required in order to obtain these potential surfaces with sufficiently high accuracy (Ref. 4).

In collaboration with Dr. R. J. Bartlett (The Johns Hopkins University and, subsequently, Battelle Memorial Institute), the technique of applying many-body perturbation theory to determine the structure of molecules has been developed from preliminary

small-scale low-accuracy calculations (Refs. 5 and 6) into rather large-scale calculations with which the desired "chemical" accuracy (in the range of 1 to 10 kcal/mole) has been achieved for molecular energies of several diatomic hydrides (Refs. 7 and 8). It is important that this accuracy be achieved using calculations that include only correlation effects due to pairs of electrons (two-body effects). The perturbation series is truncated after third order with higher order contributions included by means of denominator shifts (Ref. 9). In the many-body approach, the correlation energy is developed in terms of several diagrams representing the various types of interelectronic interactions (Ref. 10). Such diagrams are particularly useful for translating algebraic expressions into extremely efficient computational schemes for use on the computer (Ref. 11).

In developing the many-body methods for molecular applications, a number of aspects must be considered. One of these (Ref. 12) involves the use of modified potentials for the determination of excited state orbitals. Although it is possible to tailor these orbitals to some physical feature of the system under study by using a modified potential, it is found that the modified and standard potentials yield total electronic energies within 1 kcal/mole of one another when the perturbation calculations are performed through third order with shifted denominators. This shows that the costly integral transformation, required when a modified potential is used, can be avoided without significant sacrifice of accuracy. The high accuracy and low computer cost associated with the many-body calculations suggest that the many-body methods should be particularly valuable for the determination of potential energy surfaces corresponding to chemically reacting molecules.

Principal Investigators: D. M. Silver, M. Karplus, E. A. McCullough, Jr., N. J. Brown, and R. J. Bartlett. Dr. Silver is a senior chemist in the Theoretical Problems Group of the Research Center. Drs. Karplus, McCullough, Brown, and Bartlett are not funded by the program.

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Radiofrequency Enhanced Plasma Confinement

Plasma confinement poses a key problem to the development of nuclear reactors. The concept of enhancing confinement in magnetic mirrors by use of an RF electromagnetic field at a frequency slightly above the ion cyclotron frequency is attractive but has received relatively little study because theoretical justification has been based on adiabatic invariant approximations that break down under conditions of practical interest. This study examines an idealized situation that is solved without approximation. It is found that confinement occurs, so that the concept is valid under more general conditions than has been supposed.

Plasma and electromagnetic wave phenomena are important in DoD and civilian areas, including lasers, semiconductors, and radio propagation as well as thermonuclear fusion. The present study, carried out part-time by Dr. E. P. Gray, is a continuation of a low level of effort to maintain forefront analytical capability in areas of plasma physics and electromagnetic waves. During the present period, Dr. Gray received an invitation and an award from the U.S.-Australian Scientific Exchange Program to participate in the Workshop on Plasma Waves (Sydney, Canberra, and Adelaide, 10-18 February 1975), where he presented the results of the present study (Ref. 1). Also, Dr. Gray continues to author the annual update of progress in plasma physics for Science Year.

One of the serious difficulties that has beset attempts at using magnetic mirrors as thermonuclear reactors is the effect of the loss cone. Not only does this region of phase space act as a sink for particles that are scattered into it, but its existence distorts the particle distribution function in such a way as to drive the loss-cone instability and thereby further deplete the confined plasma. Any method that could eliminate or reduce the loss cone may therefore contribute significantly to the possibility of mirror reactors.

It has long been realized that RF electromagnetic fields suitably applied to a mirror plasma might prevent the escape of some or all of the particles in the loss cone. However, the interaction between field and plasma is inefficient except near resonance, and there the RF loss to the plasma has appeared to be intolerable.

Several years ago, Watson and Kuo-Petravic suggested a possible way out of this dilemma. They showed that by using a frequency only slightly above the largest ion cyclotron frequency encountered by a plasma ion in the mirror (i.e., at the point where it is reflected), the field-plasma interaction can be made sufficiently large without incurring RF loss to the plasma. This theory, which is based on the existence of several adiabatic invariants, was verified numerically by these authors and later by Gray (Ref. 2).

Recently the concept has been criticized by Klima (Ref. 3) and Lichtenberg (Ref. 4). They have shown that only a frequency very close to cyclotron resonance will permit mirror stoppering with an electromagnetic pressure much below the unacceptably large value it would require far from cyclotron resonance; such a close approach to cyclotron resonance, they point out, invalidates an assumption underlying the adiabatic invariance on which the theory is based.

In the present work it is shown that there are circumstances when the breakdown of the adiabatic invariant near resonance does not result in RF absorption, nor does it necessarily lead to less particle confinement. This was accomplished by devising a combination of constant magnetic field and position-dependent RF electromagnetic field for which closed-form exact solutions to the equations of motion were found. The RF field used is circularly polarized in a direction perpendicular to the static magnetic field; its strength is proportional to the distance along magnetic field lines from some null-point where it vanishes. (Such a field is approximation valid near the midplane of a cylindrical cavity of a circularly polarized standing wave.)

In such a field, the component of particle motion in the direction of the magnetic field is the superposition of two sinusoidal motions with frequencies m_+ and m_-, where

$$m_{\pm}^2 = \tfrac{1}{2}[g^2 + (1 - \Omega)^2] \pm \tfrac{1}{2}\{[g^2 + (1 - \Omega)^2]^2 - 4g^2(1 - \Omega)\}^{\frac{1}{2}} ,$$

$$g = \frac{eE_o}{\omega L} ,$$

$$\Omega = \frac{eB_o}{mc_\omega} ,$$

and e and m are the particle's charge and mass, c is the velocity of light, E_o, L, and ω are the strength, scale length, and frequency of the electromagnetic field, and B_o is the magnetic field strength. No matter how closely one approaches cyclotron resonance ($\Omega = 1$), where the adiabatic invariant breaks down, no RF energy is absorbed by the particle, and the amplitude of its oscillation does not increase significantly. This shows that Klima's and Lichtenberg's criticism is not applicable to this example.

It is clear, therefore, that the Watson/Kuo-Petravic containment concept remains valid under conditions not envisaged in its original proof, and that the criticism of the scheme by Lichtenberg and Klima, while pointing out real difficulties, cannot be regarded as proof that the method must fail. However, it has still not been ascertained conclusively whether or not near-resonance RF stoppering of magnetic mirrors can actually be made to work.

Principal Investigator: E. P. Gray. Dr. Gray is a senior physicist of the Theoretical Problems Group of the Research Center. He is also an instructor in the Evening College of The Johns Hopkins University.

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Statistical Physics of Phase Transitions

Techniques of statistical mechanics are important to the understanding, prediction, control, and utilization of many phenomena including phase transitions, interparticle forces, and material properties.

A modified Padé approximate technique is developed for studying the singularities of the thermodynamic functions at a phase transition critical point and for studying the dependence of these singularities on the nature of the forces of interaction between the constituent atoms or molecules. The method is applied to the three-dimensional Ising model of crystalline materials and leads to improved determination of critical exponents and new insight into their dependence on interparticle forces.

For several years, study of the Ising model has been particularly rewarding in elucidating the fundamental nature of phase transitions. Previous analysis of series expansion coefficients for the low-temperature compressibility exponent suggested a smooth convergence to a value different from the high-temperature exponent and thus in violation of the "universality" hypothesis. During the past year, we completed a study in which our modified Padé approximant technique was used to analyze recently available low-temperature series coefficients. The results of this study (Ref. 1) yield little change in the previously predicted values for body-centered cubic (BCC) and face-centered cubic (FCC) lattices but suggest values for the simple cubic (SC) and diamond (Dia) lattices which agree with universality. However, there remains some irregularity in the behavior for the SC and Dia lattices so that the addition of a few more terms appears warranted. Also, preliminary steps have been taken toward the development of virial expansions of the free energy of Ising models with longer range forces.

Remarkable similarities in the gas-liquid, the paramagnetic-ferromagnetic, and the disordered alloy-ordered alloy transitions suggest that, in an important sense, these diverse systems are equivalent. The inference is that the transition properties are insensitive to the detailed nature of the forces of interaction, and this has stimulated intensive study of the Ising (two discrete levels of interaction) model in which these diverse systems are mathematically equivalent. We had previously developed a

modified Padé approximant technique for inferring critical point properties of the Ising model from power series representations of the diverging thermodynamic functions (Ref. 2). Such power series are valid representations only in regions far removed from the critical point, and in extrapolating the predicted behavior to the critical point one expects, if the critical point is in error, that this will lead to an erroneous estimate of the strength of the divergence. It is customary to assume a power law type divergence, and in the modified Padé procedure the test estimate for the exponent in the power law is obtained by plotting various Padé estimates for the exponent against the corresponding Padé estimates for the critical point, and then extrapolating or interpolating a straight line fit through these points to the actual critical point, which is found independently.

The method has now been applied to the most recently available sets of power series coefficients for the free energy of two- and three-dimensional nearest-neighbor-Ising models. Estimates for the low-temperature compressibility exponent γ' are shown in Fig. 1 for four three-dimensional lattice structures. (The actual critical temperatures [indicated by vertical bars] have been inferred from the relatively well-behaved series expansions for the high-temperature compressibility.) The highest order term that is available is indicated by the number in parentheses next to each curve. The closed circles, open circles, and open diamonds correspond to results obtained by retaining, respectively, all the N known terms, all but one term, and all but two terms. The data for the SC lattice are particularly noteworthy. The estimates drawn as stars were obtained from low-order Padé approximants (obtained by terminating the series at a substantially lower value of N), and their extrapolation would suggest $\gamma' \approx 1.30$ for the SC lattice. However, when all the known terms are employed, the estimate is $\gamma'(e) = 1.255$ which is very close to the value $\gamma' = 1.25$ predicted by "universality." In general, the data for the SC and DIA lattices suggest that the addition of three or four more coefficients might lead to a significantly better estimate in those cases.

There are certain alloys and magnets which are nearest-neighbor Ising-like in their behavior very close to the critical point, but which show obvious deviations from this type of behavior as one goes further away from the critical point. It is possible that longer range forces are responsible for these deviations, and we are presently developing virial expansions for higher neighbor Ising models in order to investigate the effects of these forces.

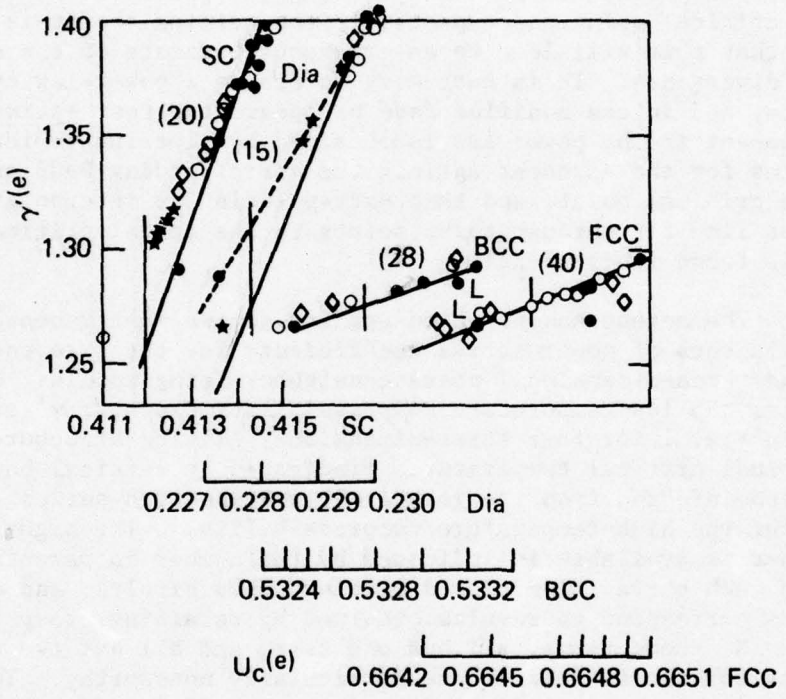

Fig. 1 Plot of the Low-Temperature Compressibility Exponent Estimates versus Corresponding Critical Temperature Estimates in the Padé Analysis of the Three-Dimensional Ising Model. The temperature variable is defined by $U_c^{(e)} = \exp(-4J/kT_c^{(e)})$, with J the exchange constant, k the Boltzmann constant, and $T_c^{(e)}$ the Padé estimate of the critical temperature. The lattice structures are body-centered cubic (BCC), face-centered cubic (FCC), simple cubic (SC), and diamond (Dia). Note that the exponent estimate for the SC lattice is extremely close to the value predicted by "universality." The dashed and solid lines for the Dia lattice indicate that γ' deduced by this method depends on which data point is chosen at low $U_c^{(e)}$.

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Principal Investigators: R. A. Farrell and P. H. E. Meijer. Dr. Farrell is a senior physicist in the Theoretical Problems Group. Dr. Meijer is Professor of Physics at the Catholic University of America and is not funded by the program.

Signal Analysis of Eye-Brain Systems

New techniques in signal processing continue to be important to science and technology, in general, and to the DoD, the Navy, and the Laboratory, in particular. Understanding of the visual system of primates (including man), viewed as a sophisticated signal processing system, offers the promise of significant new concepts. A generally applicable theory of transient signals is here verified by studies of visually evoked potentials (VEP) in the brains of monkeys. The analysis demonstrates close association of the VEP signals with an elemental response of human vision. The good agreement with predictions of the theory recommends its application to other complex systems.

The study of complex systems via signal analysis has wide-ranging application to problems of Naval and Laboratory concern. A sovereign model for complex signal-processing systems is the eye-brain system, in which light signals are processed through visual sensations into perceptual information. Thus, along with their function importance, visual systems offer a demanding testground for signal analysis.

A theory of system dynamics was developed in an abstract form that is applicable to general, complex systems. The theory postulates high-frequency linearization of a system about its dynamic steady state, from which an abrupt frequency shift is then predicted to elicit the elemental response (Green's function) characterizing the system behavior. This prediction was tested and proven by specific application to the visual system.

While there exists a massive body of visual research, little has concerned high-frequency ("suprafusion") vision. However, a novel technique using perceptual, behavioral, and neural suprafusion responses has been developed at APL for analyzing signal processing in the visual system (Ref. 1 and earlier citations therein). Recently, we have detected suprafusion electrical signals in the eyes and brains of monkeys (Ref. 2).

We report here on the analysis of VEP signals stimulated by period jumps in a luminance modulated at $\gtrsim$ 100 Hz. In brief, experiments on rhesus monkeys with electrodes implanted on their brain cortex were conducted repetitively, and the responses ensemble-averaged to bring the VEP to accurately measurable levels relative to noise. A series of such experiments with varying period jumps gave data on the behavior of the VEP transient. Analysis of the VEP signals into principal components (PC) permitted quantitative comparison with human behavioral and perceptual responses and with theoretical predictions. Further details are published in Ref. 3.

Analytical results for PC waveforms, labeled by their eigenvalues in percent signal variance, are shown in Fig. 1. Figure 1a covers the full duration of the signal, Fig. 1b the early part only. The latter analysis serves to isolate and magnify the polar (signed) PC, which is of special perceptual interest. The polar PC, though small overall (0.7%), is clearly significant in the early signal (11 to 14%).

Analysis of PC eigenvectors as a function of the experimental period jump ($t_2 - t_1$) further showed that to a good approximation all the VEP signals may be summarized into the empirical formula

$$\mathrm{VEP}(t) \tilde{\propto} (t_2 - t_1) \cdot G_{\pm}(t)$$

where $G_{\pm}$ is ($\pm$) the dominant PC, the sign depending on the sign of the jump.

We conclude from these results that the VEP signals show intimate association with suprafusion responses in man (Ref. 1). The fact that the early VEP carries a distinctive, but slight, polar component is suggestive of human perception of a definite, though elusive, polarity to the suprafusion phenomenon. Quantitatively, the close proportionality of the VEP to ($t_2 - t_1$) fits well with the psychophysical threshold value of $t_2 - t_1$ being

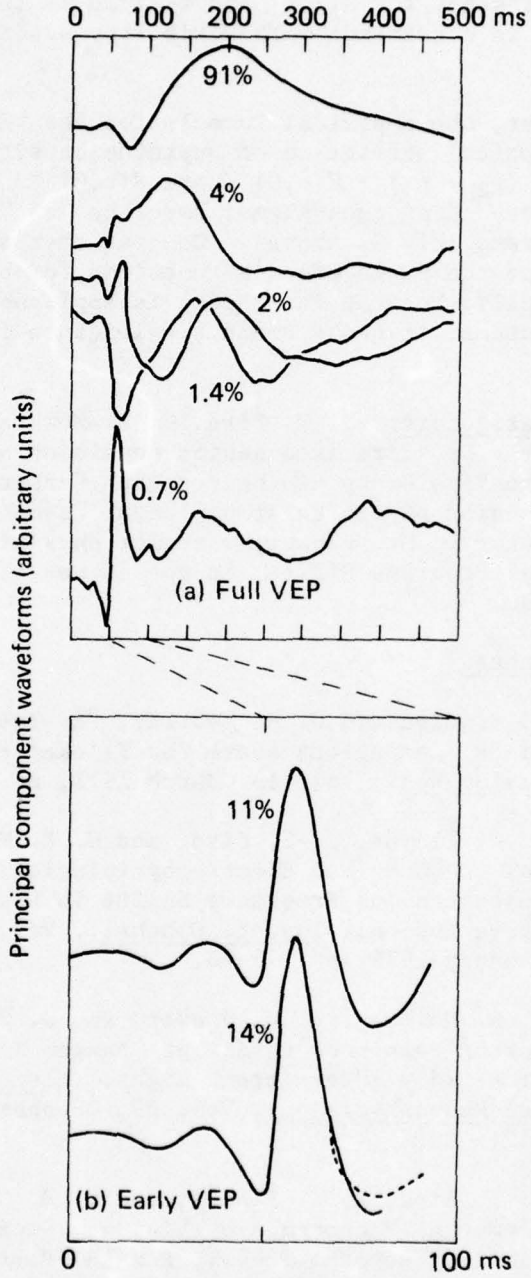

Fig. 1 Principal Component (PC) Waveforms of the Full VEP (a) and Isolation of the Polar PC of the Early VEP (b). Curves are labeled by their eigenvalues, as percentages of signal variance. Ordinates are normalized; see the text equation for amplitudes (peak $\approx 2\mu$V/ms period-jump).

accurately a constant for all t_1 and $t_2 < 10$ ms (frequencies > 100 Hz), and is consistent with visibility studies above threshold.

Further, the empirical formula for the VEP above accords with our theoretical prediction of suprafusion signals (Ref. 1), namely, $V(t) \propto (t_2 - t_1) \cdot G(t,0)$ where $G(t,0)$ is Green's function for the responding subsystems; here the "on'" and "off'" brightness systems (cf. $G_{\pm}$ above). One can then speculate on the possible role of the PC as Green's functions for brightness (Ref. 4). Finally, because the theory is applicable to other than visual systems, it bears broad significance for diverse signal analyses.

Principal Investigators: J. F. Bird, G. H. Mowbray, and R. W. Flower. Dr. Bird is a senior physicist of the Theoretical Problems Group of the Research Center. Dr. Mowbray is a senior psychologist no longer associated with the Laboratory. Mr. Flower, a senior physicist of the Biomedical Programs Office, is not supported by the IR&D program.

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Fluid Mechanics and Transport Phenomena

Advances in the mechanics of fluids continue to be of importance to a broad spectrum of Laboratory interests and to the IR&D program. In past years, Research Center investigators have made contributions in many areas, including interior and exterior ballistics of ramjet and rocket motors, combustion, heat and mass transport, and flow-separation phenomena, including biomedical applications.

Currently, the Applied Analysis component of the IR&D phase of the Research Center's activities in fluid mechanics and transport is devoted to further elucidation of flow-separation transient phenomena and to new techniques for the determination of diffusion coefficients. The two following articles describe this work. The work is carried out through the part-time efforts of Dr. C. B. Bargeron, Mr. R. L. McCally, and Dr. V. O'Brien, in collaboration with Dr. L. W. Ehrlich of the Applied Mathematics Group. Current work has been described in more detail in the publications cited in the following discussions and by several presentations at scientific meetings. Some of Dr. O'Brien's work on incompressible flows was presented by her in an invited talk for the Spring Meeting of the American Physical Society. The development of new mathematical techniques for dealing with separation and also with stratified flows (with particular application to Navy-related oceanographic problems) is carried on primarily by the Applied Mathematics Group, as described in a subsequent section of this report.

Viscous Flow Theory

Prediction of real unsteady flow is important, but difficult in many technical applications. Although the basic flow equations have long been known, complete solutions (viscous flow theory), which are dependent on geometry, wall boundary conditions, and various flow parameters, are relatively few. Through analytic and numerical simulation we have enlarged this inventory, leading insight to such phenomena as separation, porous wall boundary conditions, and phase shifts in unsteady flow. Detailed quantitative experimental verification of some unsteady simulations has been achieved.

Reliable quantitative predictive laws for laminar viscous flow problems can only be constructed by rigorous theoretical study (in contrast to gross aspects often handled semi-empirically). Fine details of model incompressible flowfields are now being

simulated by efficient finite-difference (approximate) solution of the unsteady nonlinear momentum equation (Navier-Stokes equation). Valid prediction of a real flow system by numerical simulation depends upon proper hypotheses for the mathematical boundary conditions as well as the accuracy of the numerical methods. The latter is sometimes tested by analytical solutions (where they exist), but ultimately experimental verification of a simulation (although itself inevitably limited by measurement difficulties) provides the necessary check on theoretical progress. Once the simulation is verified, a wide class of related flow problems is predicted confidently.

In some few instances of parallel flow, the details of the flow can be expressed analytically and by direct numerical approximation. One of these special cases is oscillatory flow in a straight rectangular duct. Previous published solutions were found wanting, and new analytic expressions for the harmonic flow details were derived (Refs. 1 and 2). In this geometry, any parallel unsteady flow can be synthesized by Fourier superposition or calculated by numerical time-marching.

Another tractable case of parallel unsteady flow is provided by an oscillating plate apparatus (Ref. 3) for which we can both express the viscous flow solution analytically and calculate it numerically. These flow solutions, including the induced pressure gradient, are a function of a single "Stokes number" or unsteadiness parameter, $\eta \equiv \sqrt{\omega/2\nu}\, L$ where Real part $[e^{i\omega t}]$ is the harmonic driving plate motion, ν is the Newtonian fluid kinematic viscosity, and L is the separation between the parallel plates (a fixed one and the driving one). The theoretical velocity fields (analytic and numerical approximation) and experimental measurements agree satisfactorily over a wide range of η values (Ref. 4).

Analytic steady simple shear solutions are also possible for flows parallel to a corrugated surface (Ref. 5), which are more easily (i.e., inexpensively) calculated numerically. Deep narrow corrugations provide an analog for the surface layer of an idealized porous matrix and allow the calculation of the average surface "slip velocity." These had previously been defined semi-empirically on the basis of a "slip coefficient" for certain porous surfaces. Numerical computations for parallel tangential shear flow, pressure-driven parallel flow, and pressure-driven transverse flow provide slip velocities for the same surface under various shear flows. The numerical calculations allow a critical examination of the definition and estimation of a slip coefficient (Ref. 6).

Two-dimensional Reynolds number (Re)-dependent unsteady flows have also been simulated numerically. A simple box flow reveals transient moving recirculation regions (Ref. 7) and illuminates the conditions for unsteady flow detachment (and reattachment) on a flat wall and the "breakaway" intersection of separated streamlines in midstream (Ref. 8). In all three cases, there is also a junction of a zero vorticity contour and the zero streamwise velocity component curve at the stagnation point. However, the midstream streamline intersection is orthogonal while the separating streamline may meet the wall at any angle (demonstrated analytically for certain steady Stokes flows).

Principal Investigators: V. O'Brien and L. W. Ehrlich. Dr. O'Brien is a senior physicist in the Theoretical Problems Group and Dr. Ehrlich is a senior mathematician in the Applied Mathematics Group of the Research Center.

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Laser Intensity Correlation Spectroscopy of Macromolecules

Intensity correlation spectroscopy is now the most accurate and rapid means of determining diffusion coefficients of monodisperse macromolecular particulates. This method is extended to polydisperse systems and verified by application to low and very low density lipoproteins (LDL and VLDL) of human plasma.

Improved methods for remote, noninvasive, sensing, and physical characterization of particles are important to a large variety of problem areas. In some instances, e.g., colloidal particles in the atmosphere or macromolecular and cell complexes in blood, emphasis may be placed on size and the concentration of the suspended particles themselves. In other instances, known particulates may be used to permit inferences to be drawn regarding properties (e.g., temperature) of the medium in which they are suspended.

Laser intensity correlation spectroscopy is a technique for measuring the time-dependent fluctuations in the intensity of light scattered from various media. Particles in solution scatter light, and intensity fluctuations arise from the Brownian motion of the scatterers; the decay constant of the autocorrelation function of the scattered light is related to the molecular diffusion coefficient. The diffusion coefficient is, in turn, related to the frictional coefficient by the Stokes-Einstein equation. Thus, the effective hydrodynamic diameter of scatterers can be determined from intensity correlation spectroscopy, and it is now the most accurate and rapid means for determining this important property.

The interpretation of data from polydisperse samples is complex; however, recent advances in data analysis have made the investigation of such systems practical. The cumulant method (Ref. 1) is a completely general approach to the study of polydisperse systems. Cumulant analysis yields the so-called z-average diffusion coefficient, its variance, and, in ideal cases or with sufficiently noise-free data, a third parameter related to the skewness of the generalized distribution of diffusion coefficients.

During the present period, we have applied this method to LDL and VLDL of human plasma. Plasma lipoproteins are macromolecular complexes of lipid and protein which enable the transport of normally insoluble lipids throughout the body. LDL and VLDL are the principal carriers of cholesterol and triglycerides, respectively, and are of considerable interest because of their

possible involvement in atherosclerosis. In current practice, lipoproteins are defined by their flotation properties in the ultracentrifuge. LDL comprise those lipoproteins in the density range of 1.019 to 1.063 g/cm^3 and VLDL are those having densities less than 1.006 g/cm^3 (excluding the transient species called chylomicrons that appear shortly after eating and disappear within a few hours). In the electron microscope, LDL diameters range between 21.0 and 25.0 nm and VLDL have very broadly distributed diameters ranging between 30.0 and 80.0 nm.

Pure lipoprotein samples were provided by Dr. S. Margolis of the Johns Hopkins Medical Institutions for our study, using the intensity correlation technique. Preliminary results on LDL and VLDL were reported to the Biophysical Society (Ref. 2). We find that the diameters computed from the z-average diffusion coefficients of both LDL and VLDL are in general agreement with the diameters reported in electron microscopic studies, being 24.0 and 71.0 nm, respectively. Additionally, these studies suggest a much broader size distribution for LDL than is indicated by electron microscopy. One possibility is that larger aggregates (oligomers) are present. Indeed, our preliminary data show that the z-average diffusion coefficient of LDL increases and its variance decreases with decreasing concentration. This behavior is indicative of both a smaller average particle size and a narrower distribution at smaller concentrations and is consistent with the occurrence of an equilibrium reaction between LDL monomers and LDL oligomers.

We also investigated the possibility of specifying a form for the size distributions and then using the light scattering data to predict the parameters that describe this function. Up to now, analytical techniques have been developed only for finding the parameters of a Gaussian size distribution from the values of the cumulants (Ref. 3). In the case of VLDL, our data yield a reasonable value for the center of the Gaussian, but its width is much too great to describe the known range of VLDL diameters. Our LDL data could not have resulted from a Gaussian distribution of diameters. We conclude that, for this approach to be useful in lipoprotein research, other distributional forms will be required to describe VLDL and LDL sizes. Nevertheless, the cumulant approach is valid even in the absence of knowledge of the distribution form.

Principal Investigators: R. L. McCally and C. B. Bargeron. Mr. McCally is an associate physicist in the Theoretical Problems Group and Dr. Bargeron is a senior physicist in the Electronic Physics Group of the Research Center.

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APPLIED MATHEMATICS

The Applied Mathematics Group specializes in areas of classical and modern analysis of concern to the Laboratory. The group supports various Laboratory programs, but the major portion of its work is in support of and funded by the Research Center's IR&D program. The group is made up of four senior mathematicians, each recognized as a significant contributor to his field through his published original researches. In general, active areas include numerical analysis and the development of computational algorithms, analysis of the behavior and of approximation of solutions to partial differential equations, and the development of estimation techniques in spectral theory. Applications have included improved computational procedures in numerous program areas, particularly those involving structural and fluid mechanics.

The present year has been especially notable for the inception of stratified flow studies and the early achievement of important results. Significant progress also has been achieved in the continued development of general approximation methods in differential equations and estimation techniques in spectral theory. Results are described in detail in three papers which have been accepted for publication. It is also noteworthy that Dr. D. W. Fox, Supervisor of the Applied Mathematics Group, was invited by The Johns Hopkins University to accept an appointment as William S. Parsons Visiting Professor in the Department of Mathematical Sciences for the academic year 1976-1977 and was an invited lecturer at the J. M. Jauch Memorial Workshop in Mathematical Physics held in Geneva, Switzerland, in the summer of 1975.

A Fundamental Solution for Stratified Fluid Flows

A frequently used model for the flow of stratified fluids acted on by gravity can be described by a coupled pair of second-order partial differential equations in space and time. For this system, we have found the fundamental solution in three dimensions and a solution for a general inhomogeneous initial value problem in terms of the fundamental solution. The importance of the fundamental solution is that it reduces the solution of a large class of important problems for these equations to integration.

The study of problems in the theory of stratified fluids is motivated by a need to understand the behavior of atmospheric and oceanographic flows in which the stratification and gravity introduce significant buoyant forces. When a fluid of variable density is acted on by gravity, the displacement of the heavier

fluid by the lighter brings buoyant forces into play, and the movement of such a stratified fluid is also properly called a buoyant flow. Among such flows of practical interest are the induced movements caused by the displacement of submerged bodies in the ocean, which is a slightly stratified fluid.

Although buoyant flows have been widely investigated by hydrodynamicists for many years, only the simplest problems have been solved and phenomena have remained poorly understood. It appears, therefore, that systematic mathematical techniques, including the use of fundamental solutions, should provide valuable new insights. Thus, during this reporting period a project was initiated to bring such techniques to bear.

When the equations of motion for an inviscid incompressible slightly stratified fluid are linearized about static equilibrium, the introduction of a potential for the horizontal velocity allows the system of equations to be reduced to a convenient pair of second-order equations. Under the usual hypotheses — constant buoyancy frequency and inertial density — we have found an *explicit expression* for the fundamental solution of this system of equations and its interpretation as the effect of impulsive injection of fluid into a fluid at rest.

The importance of a fundamental solution derives from the fact that, for the equations and region for which it is valid, it reduces the solution of a great variety of inhomogeneous initial-value problems to integration. Further, by a variety of more-or-less standard devices it often can be modified to apply to a number of other regions. Equally important, analysis of the behavior of a fundamental solution yields considerable information on the properties of whole classes of solutions, any of which might otherwise be difficult to obtain explicitly. In addition, it is a usual starting point for a formulation of initial-boundary-value problems in terms of integral equations.

The structure of the fundamental solution shows a natural decomposition of the flow into two parts, one the flow of nonbuoyant ideal fluid of constant density and the other a modification that gives the influence of buoyancy. The first part responds immediately to the impulsive injection, the second is slow and long lasting. We give especially simple expressions for the fundamental solution directly above and below the singular point and in the horizontal plane with it.

The solutions of the initial-value problem are then examined in light of the properties of the fundamental solution. We

note that, in addition to an oscillating source-like (injection) effect, the initial conditions produce a term that decays with time without changing its spatial distribution. Under certain conditions, this can be the total effect of the initial conditions. In other circumstances, when the initial conditions are confined to a bounded region, we show that the influence of the initial conditions dies off at large distances faster than that of a source distribution with nonzero total strength.

Principal Investigator: D. W. Fox. Dr. Fox is Supervisor of the Applied Mathematics Group of the Research Center. He is the recipient of the Scientific Achievement Award in Mathematics of the Washington Academy of Sciences and a Fellow of the Academy.

Numerical Solutions of Partial Differential Equations

The application of the conjugate gradient method to the iterative solution of large linear systems has led to a technique that appears to have great promise.

A standard technique for solving differential equations is the replacement of the partial derivative with difference quotients, imbedding the regions in a grid or network of points and applying the difference equations at each grid point. This leads to a large sparse system of algebraic equations. If the original differential system is second order, linear, and separable, the resulting algebraic system can be solved by direct methods. In most other cases, iterative methods are needed. To use these iterative methods efficiently, one must estimate a relaxation factor, which in turn requires an estimation of the largest eigenvalue of the linear system.

The conjugate gradient method, on the other hand, does not require a relaxation factor. Indeed, it essentially determines the eigenvalue distribution as it iterates.

Current techniques for solving the biharmonic equation use a relaxation method that requires (a) the decomposition of the biharmonic equation into a coupled pair of harmonic equations and (b) an estimation of the largest eigenvalue with which to compute the relaxation factor (Ref. 1). Use of the conjugate gradient method avoids both requirements. The biharmonic matrix is split into the sum of two matrices and the gradient method applied to the resulting system. Because the relevant matrix has a single dominant eigenvalue, the gradient method converges rapidly.

Current investigation centers around applying this method to other problems.

Principal Investigator: L. W. Ehrlich. Dr. Ehrlich is a senior mathematician of the Applied Mathematics Group of the Research Center. He taught two courses at the Evening College of The Johns Hopkins University for the Academic year 1974-1975.

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Approximating Solutions of a Biharmonic Boundary Value Problem

The biharmonic operator

$$\Delta^2 u = \frac{\partial^4 u}{\partial x^4} + 2\,\frac{\partial^4 u}{\partial x^2 \partial y^2} + \frac{\partial^4 u}{\partial y^4}$$

plays a prominent role in many fluid mechanics and elasticity problems, e.g., the theory of plate deformation used in the structural analysis of ship hulls. Unfortunately, the boundary value problems associated with the operator are not solvable exactly except for a few special cases, and approximation methods must be resorted to. The numerical method developed here has two advantages over many other methods: (a) it is applicable over regions of very general shape, and (b) it is the only method for which error bounds are computable.

The method depends on the existence of certain a priori inequalities (Ref. 1); their use will now be briefly outlined. We start with an appropriate a priori inequality, which for the present boundary value problem is stated by

$$\int_D v^2\,dx\,dy \le \alpha_1 \int_D (\Delta^2 v)^2\,dx\,dy + \alpha_2 \int_{\partial D} v^2\,d\sigma + \alpha_3 \int_{\partial D} \left(\frac{\partial v}{\partial s}\right)^2 d\sigma + \alpha_4 \int_{\partial D} \left(\frac{\partial v}{\partial s}\right)^2 d\sigma\ , \tag{1}$$

where $v = v(x,y)$ is an arbitrary but sufficiently differentiable function. Notice that the first three integrals on the right are in terms of data of the boundary value problem,

$$\begin{aligned} \Delta^2 u &= f_1 \quad , \quad \text{in} \quad D \ , \\ u &= f_2 \quad , \quad \text{on} \quad \partial D \ , \\ \frac{\partial u}{\partial n} &= f_3 \quad , \quad \text{on} \quad \partial D \ , \end{aligned} \tag{2}$$

while the last integral is in terms of the tangential derivative of the given boundary data. If we now denote the solution of (2) by u and construct an approximate solution u_a by

$$u_a = \sum_{i=1}^{n} a_i \phi_i \ , \tag{3}$$

where the ϕ_i are a suitable set of approximating functions, then setting $v = u - u_a$ we have

$$\begin{aligned} \int_D (u - u_a)^2 \, dx \, dy \le \alpha_1 \int_D \left(f_1 - \sum_{i=1}^{n} a_i \Delta^2 \phi_i \right)^2 dx \, dy + \alpha_2 \int_{\partial D} (f_2 - u_a)^2 \, d\sigma \\ + \alpha_3 \int_{\partial D} \left(f_3 - \frac{\partial u_a}{\partial n} \right)^2 d\sigma + \alpha_4 \int_{\partial D} \left(\frac{\partial f_2}{\partial s} - \frac{\partial u_a}{\partial s} \right)^2 d\sigma \ . \end{aligned} \tag{4}$$

Thus we have a norm error bound on the approximation u_a to u in terms of the undetermined coefficients a_i, $i = 1,2,\ldots,n$. The a_i that minimize the right hand side of (4) are found by solving the linear system:

$$\sum_{k=1}^{n} a_k \{\alpha_1 \int_D \Delta^2\phi_k \Delta^2\phi_i dx + \alpha_2 \int_{\partial D} \phi_k\phi_i \, d\sigma + \alpha_3 \int_{\partial D} \partial\phi_k/\partial n \cdot \partial\phi_i/\partial n \, d\sigma$$

$$+ \alpha_4 \int_{\partial D} \partial\phi_k/\phi s \cdot \partial\phi_i/\partial s \, d\sigma\} = \alpha_1 \int_D f_1 \Delta^2\phi_i dx \qquad (5)$$

$$+ \alpha_2 \int_{\partial D} f_2\phi_i d\sigma + \alpha_3 \int_{\partial D} f_3 \partial\phi_i/\partial n \, d\sigma$$

$$+ \alpha_4 \int_{\partial D} \partial f_2/\partial s \cdot \partial\phi_i/\partial s \, d\sigma \quad ,$$

$$i = 1,2,\ldots,n$$

The inequality (1) has been used to calculate approximate solutions for a group to test functions over rectangles, triangles, and circular sectors. The results indicate that the method can indeed yield quite good approximations with maximum relative errors of the order of 10^{-6} to 10^{-7}. A more detailed discussion of the method and results of the test examples are given in Ref. 2.

Principal Investigator: V. G. Sigillito. Dr. Sigillito is a senior mathematician of the Applied Mathematics Group of the Research Center. He was the instructor for two courses at the Evening College of The Johns Hopkins University for the academic year 1974-1975.

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Estimating Frequencies of Differential Operators

A method is given for estimating points in the spectrum of a general self-adjoint elliptic partial differential operator. Given rough preliminary estimates on their location, the method systematically employs arbitrary trial functions to give both upper and lower bounds.

Eigenvalue problems associated with certain elliptic partial differential operators are of significant interest in naval structural mechanical applications because, among other things, the eigenvalues of such problems are proportional to the frequencies of the vibration of membranes and plates. Often, however, only crude bounds are known for the eigenvalues and more refined estimates are needed for design purposes. Given rough preliminary estimates of the eigenvalues, the method presented here can be used to give refined estimates through improved upper and lower bounds for the eigenvalues. The unique feature of the method is that the trial functions used to obtain the bound can be quite arbitrary and need not satisfy the boundary conditions of the problem.

We present the method in the setting of a symmetric operator in a Hilbert space to preserve and illustrate the general applicability of the method. Those readers unfamiliar with this approach would probably gain a clearer understanding by thinking of a concrete representation of the operator A (defined below), for instance as the Laplacian with zero boundary conditions. Central to the method is the combination of the a posteriori inequality (1) with the a priori inequality (3) to produce the bound (4).

Suppose, then, that A is a symmetric operator on a domain $\mathfrak{D}(A)$ dense in a separable Hilbert space H, and that A has pure point spectrum $\{\lambda_i\}$ with corresponding orthonormal eigenvectors $\{u_i\}$ that are complete in H. Let A_* be an invertible extension of A (i.e., $\mathfrak{D}(A) \subset \mathfrak{D}(A^*) \subset H$ with $A_* u = Au$ for $u \in \mathfrak{D}(A)$). Then, if there exists a function w satisfying

$$A_* w = A_* u_* - \lambda_* u_* \quad , \quad u_* - w \in \mathfrak{D}(A) \ , \tag{1}$$

then for any number λ_* and any function $u_* \in \mathfrak{D}(A)$,

$$\min_i \left| \frac{\lambda_* - \lambda_i}{\lambda_i} \right| \leq \frac{\| w \|}{\| u_* \|} \tag{2}$$

Now the inequality (1) is combined with an a priori estimate for w in terms of u. For example, suppose R is a body with boundary ∂R, the Hilbert space is $\mathcal{L}_2(R)$, and the operator is the negative Laplacian $-\Delta$ on R, with domain consisting of the twice-differentiable functions on R that vanish on ∂R. The inequality a priori applicable is

$$\left(\int_R w^2\,dx\right)^{\frac{1}{2}} \le C_1\left(\int_R (\Delta w)^2\,dx\right)^{\frac{1}{2}} + C_2\left(\oint_{\partial R} w^2\,ds\right)^{\frac{1}{2}} . \qquad (3)$$

where C_1, C_2 are explicitly computable constants depending only on R (see Ref. 1). Putting (3) into (1) and using (2) yields

$$\min_i \left|\frac{\lambda_* - \lambda_i}{\lambda_i}\right| \le \frac{C_1\left(\int_R (\Delta u_* + \lambda_* u_*)^2\,dx\right)^{\frac{1}{2}} + C_2\left(\oint_{\partial R} u_*^2\,ds\right)^{\frac{1}{2}}}{\left(\int_R u_*^2\,dx\right)^{\frac{1}{2}}} .$$

Squaring and using Schwarz's inequality gives

$$\min_i \left|\frac{\lambda_* - \lambda_i}{\lambda_i}\right|^2 \le \frac{2C_1^2 \int_R (\Delta u_* + \lambda_* u_*)^2\,dx + 2C_2^2 \oint_{\partial R} u_*^2\,ds}{\int_R u_*^2\,dx} . \qquad (4)$$

Now let $u_1, u_2, \ldots, u_n$ be arbitrary test functions that are twice-differentiable. Let $u_* = a_1u_1 + a_2u_2 + \ldots + a_nu_n$ and let λ_* be a guess for an eigenvalue. Now minimize the right side of (4) with respect to the undetermined coefficients a_i as in the Rayleigh-Ritz method. The minimum is ε^2, the smallest eigenvalue of the relative matrix eigenvalue problem

$$Aa - \varepsilon^2 Ba = 0 ,$$

where the matrices A and B are defined by

$$A_{ij} = 2C_1^2 \int_R (\Delta u_i + \lambda_* u_i)(\Delta u_j + \lambda_* u_j)\,dx + 2C_2^2 \oint_{\partial R} u_i u_j\,ds ,$$

$$B_{ij} = \int_R u_i u_j\,dx ,$$

and the vector a is the transpose of $(a_1,\ldots,a_n)$. The more test functions that are used, the smaller ϵ^2 will be. The minimizing value u_* can be used to find an improved guess λ_* for the eigenvalue. Details are given in Ref. 2.

Principal Investigators: J. R. Kuttler and V. G. Sigillito. Dr. Kuttler and Dr. Sigillito are senior mathematicians in the Applied Mathematics Group of the Research Center. Dr. Kuttler was an instructor at the University College (Evening College) of the University of Maryland from September 1974 through December 1974.

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1. J. R. Kuttler and V. G. Siggillito, "Inequalities for Membrane and Stekloff Eigenvalues," J. Math. Anal. Appl., Vol. 23, 1968, pp. 148-160.

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ATOMIC, MOLECULAR, AND ELECTRONIC PHYSICS

Improved basic understanding of energy levels and energy-transfer mechanisms continually leads to new technological capabilities in a very wide variety of areas, including lasers, computers, electromagnetic detectors, and rocketry. Fundamental research in atomic, molecular, and electronic physics continues to be a fruitful component of the Research Center's IR&D program. Emphasis is placed on the development of techniques and basic understanding with respect to energy states and energy-transfer mechanisms.

In the past year, the Electronic Physics Group has made significant progress on a variety of research studies in atomic, molecular, and electronic physics. Six publications appeared in the literature during this period and others are now in preparation. Present studies include (a) mass spectrometry of highly reactive species, (b) scanning electron microscopy, (c) acoustic waves in cavities and crystals, and (d) hyperfine structure constants of halogen molecule ions.

The work carried out on each of these topics is summarized in the attached individual research reports. In addition, the Electronic Physics Group has for many years been involved in electron spin resonance studies of free radicals in collaboration with the Microwave Physics Group. Work on this topic is included in the IR&D report of the Microwave Physics Group.

Mass Spectrometry of Highly Reactive Species

Atomic fluorine reactions of the type (R-H) + F → R + HF have been studied in the crossed molecular beam reactor. These are found to be a rich source of free radicals. The hydrogen fluoride product is sometimes left in a highly excited state.

The identification and characterization of highly reactive chemical species (e.g., free radicals and excited molecules) are fundamental to the understanding of a great variety of chemical and laser systems. Molecular beam techniques provide a unique means of carrying out such studies under particularly well-defined conditions. The Laboratory has pioneered in the development and use of molecular beam techniques for the study of fundamental chemical reactions. The work has achieved wide recognition; during the present year, Dr. S. N. Foner, Supervisor of the Electronic Physics Group, was invited to prepare for publication the early

personal reminiscences on molecular beam research of the late Dr. Immanuel Estermann (Ref. 1).

Emphasis in present research with crossed molecular beams is being placed on reactions involving fluorine. The reactions of fluorine atoms are of current interest because they have not been as intensively studied as reactions involving more tractable materials, and the large amounts of energy released in reactions with hydrogenous compounds suggests potential applicability in the fields of high-energy fuels and chemical lasers. The crossed molecular beam inlet system of the APL mass spectrometer (Ref. 2) provides a unique method for directly observing the products of elementary reactions. In some cases it is possible to determine whether a product is in an electronically excited state, which relates to laser applications as well as to chemical kinetic theory.

Bimolecular reactions of the type $X + F \rightarrow R + HF$ where R = radical and X = (R-H) are currently being studied.

Fluorine, diluted by a carrier gas of helium and/or argon, flows through a 0.5-in.-diameter alumina tube at reduced pressure. Immediately before reaching the molecular beam entrance orifice, it passes through a 2450-MHz electrodeless microwave discharge, where the fluorine is more than 99% dissociated. The reactant X is introduced via a molecular beam just behind the entrance orifice. Table 1 gives a list of reactions that have been observed, together with values for the theoretical energy release.

The occurrence of the radicals CH_3 and NH_2 in the reactant column is a consequence of their high production rate in initial reactions. Their subsequent reactions with F atoms produce secondary products in small but observable quantities. Ionization potential measurements were obtained for all radicals listed in Table 1 except C_2H and H, which had low intensities. The low level of the hydrogen atom signal may be the result of momentum conservation and the consequent low density of the atoms because of their high velocity if a substantial part of the reaction energy is converted to kinetic energy. However, the low density of C_2H radicals is probably due to a relatively low reaction rate, although any reaction observed by this technique must be considered to be moderately fast.

Measurements of the ionization potential of the HF reaction product indicate that it is sometimes left with substantial excitation energy. The onset energy for HF^+ from the reactions

Table 1

Atomic Fluorine Reactions

Reactant X	Radical Product R	Energy Release ΔH (kcal/mole)
$n - C_4H_{10}$	$n - C_4H_9$	35.0
$n - C_4H_{10}$	$sec - C_4H_9$	44.7
CH_4	CH_3	30.6
CH_3	CH_2	23.2
C_2H_2	C_2H	25.9
NH_3	NH_2	31.7
NH_2	NH	45.7
H_2O	OH	16.6
H_2	H	31.6

$$NH_3 + F \rightarrow NH_2 + HF$$

and

$$C_4H_{10} + F \rightarrow C_4H_9 + HF$$

occurred about 0.6 eV (13.8 kcal/mole) and 1.0 eV (23.1 kcal/mole), respectively, below the ionization potential of 15.77 V for the ground state molecule. This energy accounts for about half the total heat of reaction in each case.

Figure 1 shows the de-Boltzmannized ionization curve of HF from the reaction with ammonia, together with that of the argon reference gas. The sharp upward break at about 15.8 V indicated in the figure by the arrow probably represents ions produced from ground state molecules, while the curve below that point results from metastable molecules.

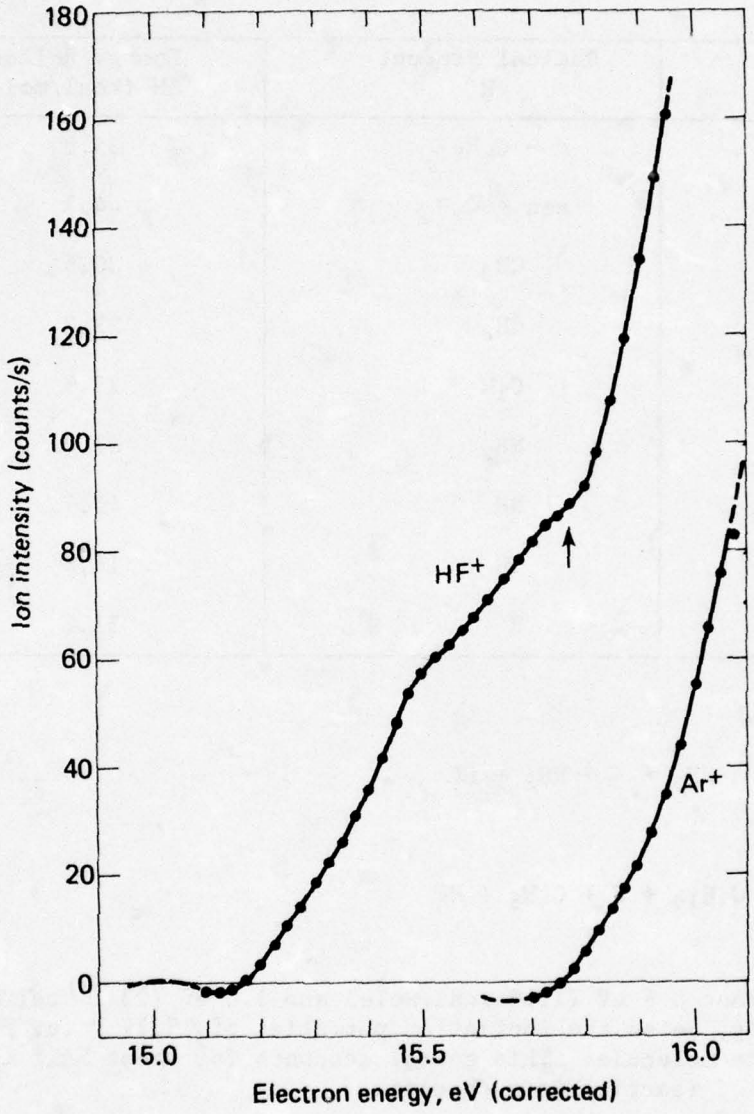

Fig. 1 De-Boltzmannized Ionization Curve Showing Metastable Hydrogen Fluoride Produced by Reacting Fluorine Atoms with Ammonia. The energy scale has been corrected for instrumental shifts by using argon as a reference standard.

Principal Investigators: S. N. Foner and R. L. Hudson. Dr. Foner is the Supervisor and Mr. Hudson is a senior engineer of the Electronic Physics Group of the Research Center.

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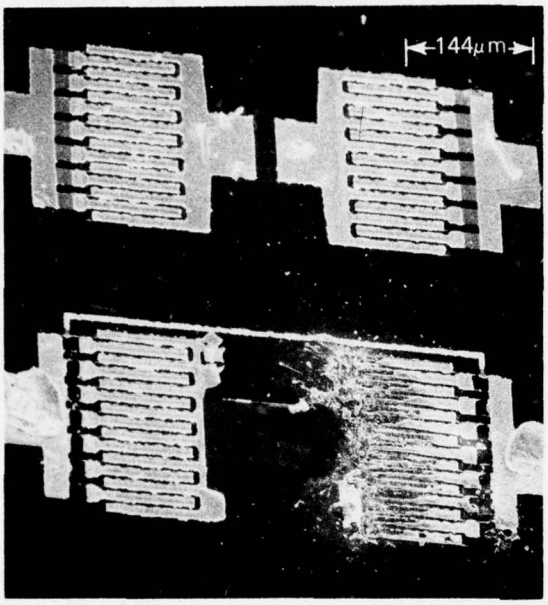
Scanning Electron Microscopy

The scanning electron microscope has been used to study the topography and chemistry of solid surfaces and to analyze important features of a variety of microcomponents.

The recently acquired scanning electron microscope (SEM) has a magnification range of 5 to 240 000 and a spatial resolution of about 7 nm. With its energy-dispersive X-ray accessory system, it can provide elemental analysis of surface composition with a spatial resolution of about 100 nm. The ultra-high-vacuum pumping system on this instrument eliminates the possibility of contamination of the samples by ambient background gases, particularly pump oil, thereby making it feasible to carry out physical and chemical research on clean surfaces.

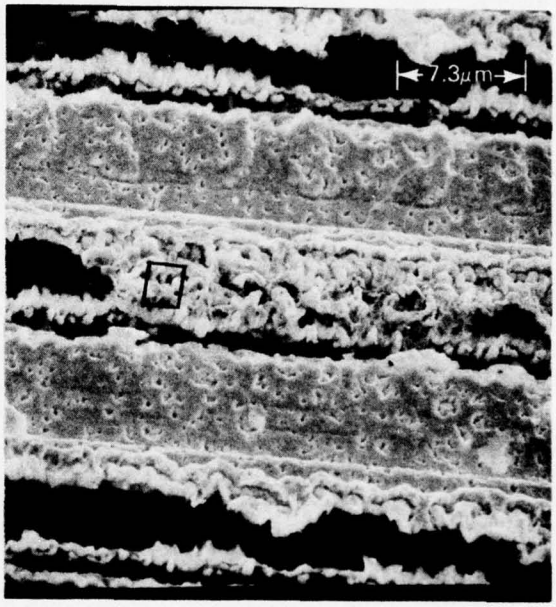
The SEM arrived in late March 1975, and the X-ray analysis accessory system came in May. A considerable effort was dedicated to setting up the instrument, determining its characteristics, optimizing operational parameters, and learning specialized SEM techniques.

The investigations carried out with the SEM have ranged from research on the surface structure of thin films of amorphous semiconductors and electron breakdown effects in boron switching capacitors to secondary electron and X-ray analysis of the causes of failure in microelectronic devices. During this period, samples analyzed included 19 electronic packages such as integrated circuits transistors and other microelectronic components, 13 samples of thin-film amorphous semiconductors and switching capacitors, and 4 sets of organic crystals which are one-dimensional conductors.



140x

Fig. 1a Overall View of a High-Frequency Transistor from a Transit Improvement Program II Satellite



2800x

Fig. 1b Close-Up of Extraneous Matter between the Gold Electrode Fingers. The small outlined area was analyzed for elemental content by detecting emitted X rays

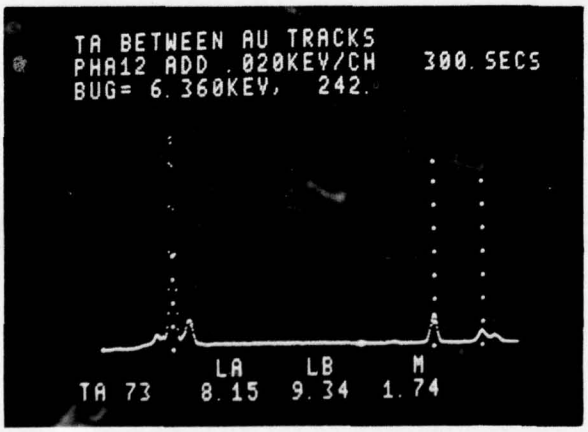
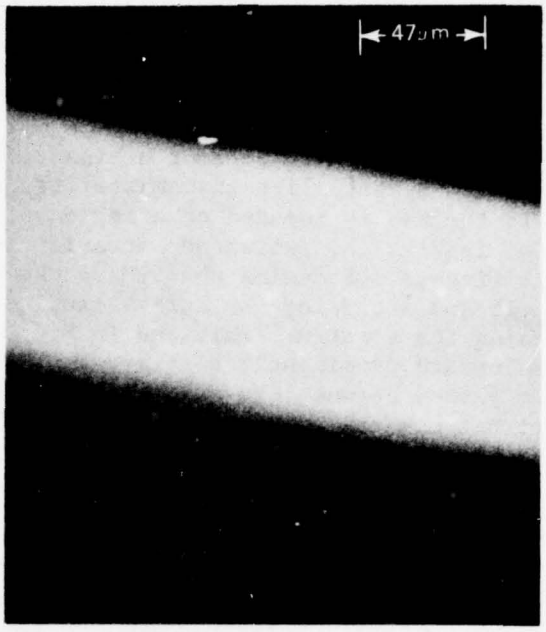
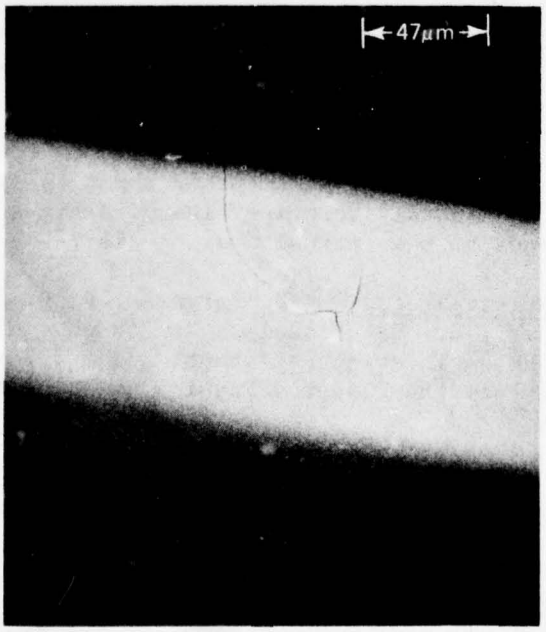


Fig. 1c X-ray Spectrum of Outlined Region in Fig. 1b. The lines of tantalum are very prominent



440x

Fig. 2a A Thin Film Capacitor Consisting of a 1 μm Boron Film between Two 0.25-μm Titanium Electrodes



440x

Fig. 2b The Capacitor after a Single 2.5-ms Switching Pulse of 20 V Amplitude Was Applied

Some of the analytical capabilities of the SEM are illustrated by the following examples from these studies.

An important application of scanning electron microscopy is in the evaluation of microelectronic components and in the definitive analysis of the mechanisms responsible for failure. As an example, consider the failure of a high-frequency Transit Improvement Program II satellite transmitter transistor, as shown in Fig. 1a. If the SEM is focused on a region of undamaged transistor as shown in Fig. 1b, extraneous material is observed between the gold fingers. Focusing the SEM on the small region outlined in Fig. 1b and analyzing the X rays excited by the electron beam, one obtains the spectrum exhibited in Fig. 1c in which the lines of tantalum are prominently displayed. This indicates that tantalum had migrated between the gold fingers and, probably, caused a short between the emitter and base electrodes of the transistor, resulting in the massive damage seen in Fig. 1a.

Another example that provides information on the physical mechanism of electrical breakdown is the observation in the microscope of the effect of applying a voltage pulse to a thin-film boron switching capacitor. Figure 2a shows a capacitor before a single electrical switching pulse was applied to the electrodes via a multipin electrical feedthrough into the chamber. Figure 2b shows the capacitor after a single 2.5-ms pulse of 20 V. The exceptional resolution of this and other pictures of the surface permitted observations of microcracking that are not detectable with an optical microscope. The results of these studies, which clearly localize the breakdown regions, tend to substantiate the electrothermal model for switching in these films (see the section on Solid State Physics of this report).

A number of research applications of the SEM to the study of physical and chemical phenomena on surfaces are being investigated, including catalytic properties of various materials and several aspects of the corrosion of metals.

Principal Investigators: C. B. Bargeron, R. B. Givens, and S. N. Foner. Dr. Bargeron is a senior physicist, Mr. Givens is an engineering assistant, and Dr. Foner is the Supervisor of the Electron Physics Group of the Research Center.

Acoustic Waves in Cavities and Crystals

Viscous acoustic damping by large particles was found, in accord with theory, to depend upon body shape. A disk placed edge-on attenuates less than a sphere of the same area, while a

fine mesh screen placed broadside attenuates more than a sphere by a factor of 14. Initial experimental studies of surface-wave-to-bulk-wave conversion at the ends of rectangularly cut crystals of anisotropic materials commonly used for surface wave devices have shown that the largest bulk wave generated on reflection-conversion in Y-cut, Z-propagating $LiNbO_3$ is a shear wave beam with a forward component of direction. In certain crystal orientations there is a common path for end-generated compressional and shear wave energy flow.

Acoustic Damping by Particulates in Cases

The absorption of sound by small particles continues to be of interest in connection with the stability of rocket motors. Previous studies of the thermal and viscous damping of spheres in an acoustic field (Ref. 1), showing good agreement between experiment and theory, were published during the present year (Ref. 2).

During the present year, further experiments were performed to determine the effect of particle shape on viscous and thermal damping. The result for large particles is that thermal damping is a function of body area, not of shape. On the other hand, Kanwal (Ref. 3) has made a theoretical study of the effects of body shape upon the drag (which produces viscous damping) experienced by the body in slow vibration in a fluid along an axis of symmetry. For equal body areas, his theory gives the drag ratio (damping ratio): disk broadside/disk edge-on/sphere as 9.60/5.23/6.0. We have performed a single experiment at APL giving the viscous damping ratio for the three cases as 10.2/5.7/6.0, in good agreement with Kanwal's theory.

Other experiments were performed toward the goal of maximizing viscous damping with the result that fine screens (300 mesh and 400 mesh) of surface area equal to that of a 0.95-cm-diameter sphere produce 14 times as much damping at 1200 Hz.

The large viscous damping property of small disks of the fine screen suggests possible uses in rocket motors that are marginally stable to acoustic oscillation. In these cases, the burning propellant gases must not contain particles. The screen disks should be placed broadside to the particular acoustic particle motion of concern.

Bulkwave Generation in Surface Wave Crystals

The study of bulk wave generation in surface wave crystals (Ref. 4) continues and has now been extended to include surface-

wave-to-bulk-wave conversion at the rectangularly cut and polished ends of crystals. While some of this work is preliminary, the experiments already show several interesting results. For example, interdigital transducers launch the Rayleigh surface acoustic wave bilaterally with equal efficiency in both directions even in an anistropic material. On the other hand, particularly in the widely used Y-cut, Z-propagating $LiNbO_3$, the conversion of surface waves to bulk waves at the crystal ends appears to be about 20-fold greater for the shear wave with a forward direction component than for that with a backward direction component. This implies that suppression by absorption of the backward traveling Rayleigh wave would eliminate the largest single bulk wave produced in a Y-cut $LiNbO_3$ crystal.

A second feature of note is that, in both Y-cut, Z-propagating and X-cut, Z-propagating $LiNbO_3$ and in X-cut, Y-propagating quartz, there are vertical shear beams and compressional wave beams that are reflected along the same path in the crystal. For anisotropic materials, this is clearly an unexpected result since the compressional velocity depends upon different elastic moduli than those that determine shear wave propagation.

Principal Investigator: B. H. Nall. Mr. Nall is a senior engineer of the Electron Physics Group of the Research Center.

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Hyperfine Structure Constants of Halogen Molecule Anions from Spin-Correlated Valence Bond Wave Functions

An approximate valence bond (VB) wave function that includes correlation between electrons of opposite spin is used to interpret the experimental hyperfine structure (hfs) and electronic g-factor data for the halogen-molecular anions $(XY)^-$ in terms of the internuclear distance and charge distribution of these molecules. It was found that interatomic correlation and the inclusion of both the valence and inner shell s electrons are important factors in the determination of the isotropic hfs constants. The estimates of internuclear separation and charge distribution obtained are consistent with considerations of ion sizes and electronegativities.

Theoretical studies of structure at the atomic/molecular level have continued. The interpretation of fine and hyperfine structure in metastable states of molecular hydrogen described in the FY 74 IR&D report (Ref. 1) have now been published (Refs. 2 and 3). During the present reporting period, emphasis in theoretical analysis has been placed on the study of defect centers in alkali halides.

The study of defect centers in the alkali halides has received renewed interest recently since there is a possibility that their anisotropic optical absorption properties can be exploited as memory devices in computer applications. One class of such defects is the V_K center or halogen-molecule anion $(XY)^-$ formed and stabilized at low temperatures in an alkali halide lattice. This work is an extension of our earlier work (Ref. 4) on the optical behavior of the homonuclear molecules to the magnetic properties of both the homonuclear and heteronuclear molecule anions.

Since these molecules have an unpaired electronic spin, they are paramagnetic and exhibit a resolvable hyperfine structure caused by the interaction of the unpaired spin with the nuclear magnetic moments. The experimentally determined coupling constants are subject to theoretical analysis. Using the VB method, a semiempirical wave function was constructed of the form

$$\Psi = N\,[\varepsilon\,\Psi(X\text{--}Y^-) + \sqrt{1-\varepsilon^2}\,\Psi(X^-\text{--}Y)]$$

which includes electron correlation for the $(XY)^-$ molecules. Intra-atomic correlation is treated by using halogen atom orbitals for X and halogen anion orbitals for Y^- in VB structures $(X\text{--}Y^-)$

and vice versa in VB structures (X^---Y). Interatomic electron correlation is treated by a perturbation theory calculation of the polarization of X by Y^- in (X--Y^-) and vice versa in (X^---Y). Interatomic polarization and the requirement that orbitals on different atoms be orthogonal are the important factors in the isotropic hfs constants. It is also important to consider both the valence and inner shell s electrons.

With the spin-correlated VB wave function, the isotropic hyperfine constant A was calculated as a function of internuclear distance R and electronegativity factor ε. The electronegativity factor weighs the electronic charge distributions centered on the nuclei of the molecule ($\varepsilon = 1/\sqrt{2}$ for the homonuclear molecules). The values of R and ε were determined as those giving the best fit between the calculated and experimental A values. The anisotropic coupling constant B was then calculated and compared with the corresponding experimental quantity after the latter had been corrected for the contribution arising from spin-orbit mixing of the ground and excited states of the molecule. This correction can be related to the electronic g-factor data. The results are tabulated in Table 1.

Table 1

Comparison of Experimental and Theoretical Hyperfine Coupling Constants for the Halogen-Molecule Anion in the Alkali Halides

Substance	Exp A(MHz)	R(nm)	ε	Exp B(MHz)	Theory B(MHz)
F_2^- in KF	772.8*	0.184	0.707	1792.2*	1778.1
Cl_2^- in KCl	112.7*	0.263	0.707	175.4*	173.1
Br_2^- in KBr	448.9*	0.288	0.707	792.1*	787.7
$ClBr^-$ in KCl (Cl)	92.0**	0.278	0.661	165.0**	157.4
$ClBr^-$ in KCl (Br)	517.3**	0.275	0.750	875.5**	840.2
FCl^- in KCl (F)	566.5†	0.224	0.661	1710.3†	1634.7
FCl^- in KCl (Cl)	146.6†	0.222	0.750	211.4†	182.0
FBr^- in KBr (F)	542.6†	0.237	0.600	1476.6†	1445.4
FBr^- in KBr (Br)	594.6†	0.254	0.800	1096.1†	887.5

*Ref. 5, **Ref. 6, †Ref. 7

From this table, it is noted that a completely consistent description of the molecule-ions is achieved with the VB treatment with reasonable values for the internuclear distances. For the heteronuclear molecules, two internuclear distances are obtained depending on whether the experimental hyperfine data for X or for Y in $(XY)^-$ are used in fitting to the theoretical calculations for A. The difference between these distances can be used as an assessment on the success of the theory in addition to the comparison between the experimental and theoretical values for B. Also note that the sum of the squares of the electronegativity factors for the heteronuclear molecules add to one as a consequence of the normalization of the wave functions. The electronegativity factors are in accord with the relative electronegativities of the component atoms in the heteronuclear molecules.

Principal Investigators: F. J. Adrian and A. N. Jette. Dr. Adrian is Supervisor of the Microwave Physics Group and Dr. Jette is a senior physicist of the Electronic Physics Group of the Research Center.

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CHEMICAL PHYSICS

The objective of the Chemical Physics component of the IR&D program is to continue to provide an up-to-date advanced capability in interdisciplinary areas between chemistry and physics through innovative research on selected topics of significance.

The Chemical Physics Group has long pioneered in basic investigations of gas phase interactions between atoms, molecules, and the molecular fragments (free radicals) that are produced during gaseous reactions as the reactants are fragmented and reconstituted to form the reaction products. Early studies were an outgrowth of Laboratory programs concerned with explosives and high-speed propulsion systems and gained a widely recognized stature for the Laboratory. More recently, the first realization that the natural ozone layer of the earth can be perturbed by human activities is attributed to presentations of Dr. A. A. Westenberg (Supervisor of the Chemical Physics Group of the Research Center) and Prof. H. S. Johnston (University of California) in March 1971. Stature continues to be maintained — it is noteworthy that in September, Dr. Monchick became William S. Parsons Visiting Professor in the Chemistry Department of The Johns Hopkins University for the academic year 1975-1976. It is also significant that recognition of sophisticated acoustic techniques, developed in the course of basic research studies of intermolecular energy transfer, led to a request and directly funded support, by a nonprofit agency concerned with safety, for an ongoing study of acoustic detection and localization of gas leaks in gas distribution systems.

Current emphasis is placed in areas of combustion, laser, and pollution chemistry. Projects include the measurement of the rates of reaction between atoms, free radicals, and molecules, the rates of energy transfer between molecules, and theoretical studies of molecular collision processes. Results are described in detail in nine publications that appeared in print during the present year and two other papers that were accepted for publication.

Kinetics of Gas Phase Reactions

The fast flow reactor with electron spin resonance (ESR) detection has been used to measure the rate of the reactions $O + SO_2 + M \rightarrow SO_3 + M$, $H + CH_3X \rightarrow CH_3 + HX$, *and* $O + CH_3X \rightarrow CH_2X + OH$ *over a range of temperature and pressure.*

Practically all reactions that occur in gases involve atoms or free radicals, either reacting with each other or with stable molecules. The chemical kinetics research program undertakes the study of such elementary reaction rates under precise, well-defined conditions. The experimental approach makes use of a fast-flow system in conjunction with ESR spectroscopy for the detection of atoms and radicals and mass spectroscopy for the measurement of stable species. In this method, a stream of atoms or radicals from a suitable source is carried down a tube by the fast flow of an inert gas (such as helium). A stable reactant gas is injected into the stream, and reaction between the atom and the stable species begins. By monitoring the concentration of the atoms at a point downstream, the rate of the reaction can be determined. The use of the ESR technique for quantitatively measuring the concentration of atoms and radicals in such a system was developed and verified at the Laboratory; it is now the best single method available from the standpoint of sensitivity, versatility, and reliability. The apparatus is useful over a temperature range of 200 to 1000°K.

Research efforts during the year involved a study of the rate of the important reaction $O + SO_2 + M \rightarrow SO_3 + M$. Besides the measurements over a range of pressure required because of the termolecular nature of the reaction, it was also necessary to investigate an unusually wide range of SO_2 concentration in order to separate the effects of the inert diluent gas (He or N_2) as the third body M from that of SO_2 itself. In this way, it was established that the efficiency of SO_2 as a third body is 10 times that of He, but not more than a factor of 100 higher as had been previously supposed.

The temperature dependence of the reaction was investigated over the range 250 to 415°K, with the interesting result that the effective activation energy was found to be positive. This is an unusual feature because the rate constant for most termolecular reactions that have thus far been studied under well-defined conditions have a negative temperature coefficient (i.e., a negative "activation energy"). The reason for the opposite behavior in the $O + SO_2$ case can be traced to the spin-forbidden nature of the fundamental step. Taken in conjunction with the $O + SO_3 + M$ reaction previously investigated in our laboratory (Ref. 1), which has a normal temperature dependence, the relative rate $(O + SO_2)/(O + SO_3)$ depends strongly on the temperature. Thus, at combustion temperature one would expect appreciable SO_3 formation, while at typical atmospheric temperature SO_3 would tend to be suppressed. This conclusion is of considerable practical significance. A paper on this work has been accepted for publication (Ref. 2).

Another phase of research in this area involved measurement of the rates of the reaction $H + CH_3X \rightarrow CH_3 + HX$ (X = F, Cl, Br) and $O + CH_3X \rightarrow CH_2X + OH$, both of which are crucial to understanding the behavior of such halogenated compounds as flame inhibitors. In the former case, the data obtained up to 1000°K overlapped the temperature of actual flame experiments on this reaction performed previously in this Laboratory by an entirely different technique. This is one of the very few examples where flame and nonflame experiments have been possible at the same temperature, and the excellent agreement found was gratifying. The essential difference between the H and the O reactions is that the H is removed from the system by being tied up in HX, while the O is simply converted to the still more reactive OH radical. Thus, the inhibiting action of CH_3X effectively acts via the H rather than the O. Two papers on these reactions were published during fiscal year 1975 (Refs. 3 and 4).

Dr. Helmut Schacke, a postdoctoral fellow from the University of Göttingen in Germany, was associated with the group for 6 months during the year, during which time he was involved with experimental studies of plastic flammability.

Principal Investigators: A. A. Westenberg and N. deHaas. Dr. Westenberg is the Supervisor of the Chemical Physics Group of the Research Center. He has been awarded the Combustion Institute Silver Medal and the Hillebrand Prize of the Chemical Society of Washington. Mr. deHaas is a senior physicist of the Chemical Physics Group.

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Kinetic and Collision Theory

Gas phase transport and collisional phenomena have long been of concern in many areas, including lasers, combustion, atmospheric pollution, and aerodynamics. The study of the phenomena is being continued, and significant new results have been obtained with respect to rotational transition probabilities, line broadening, transport coefficients, and differential and integral scattering cross sections.

Two studies have been completed — one on He-CO collisions (Ref. 1) and the second on He-HCl collisions (Ref. 2) — in which a variety of collision properties were computed. These include line broadening, primarily a function of the long-range anisotropy; rotational transition probabilities, primarily a function of short-range anisotropies; and transport, differential, and integral scattering cross sections. Although all of these properties are really functions of the whole intermolecular potential, the functional dependence is particularly hard to disentangle for the last three. There are many ideas extant on how this could be done, but nothing has yet been developed in a systematic way. The aim of our project is to carry out accurate calculations on a set of representative systems modelled by realistic potentials and to predetermine how useful approximate schemes are in treating scattering processes. The two completed studies have already been able to shed some light.

In both studies, it seems that the transport coefficients are principally a function of the spherical average of the potential. Approximations based on this make for a great saving in effort in calculating transport properties and, working backward, an inversion of transport properties can thus perhaps be used to determine one component of the intermolecular potential. This is not true of integral and differential scattering cross sections in general; in particular, it is not true of He-CO collisions (see Ref. 1). But it is true of He-HCl scattering, and study shows that the difference derives from the faster rate of rotation of the HCl molecule. This suggests a criterion for the neglect of the molecular anisotropy in collision cross sections.

These calculations have been carried out for intermolecular potentials approximated by the Kim-Gordon electron gas model (Ref. 3). They can also be compared with experiment, and so can be used to test the Kim-Gordon model, an extremely fast method of calculating intermolecular potentials. Other approximate methods of solving the scattering equations are being tested for molecular collisions. So far, the results are mixed and seem to indicate that there are no widely valid shortcuts to calculating scattering properties of anisotropic molecules.

In a separate study (Ref. 4), an approximate form of the collision Ehrenfest theorem (see Ref. 5) was used to determine an approximate relation between the hardness of an intermolecular potential, defined in terms of the logarithmic derivative of the potential at an energy somewhat higher than thermal energy, and the thermal diffusion ratio. This relation is exact for inverse power potentials and very accurate for exponential repulsive potentials.

A paper was published in another field (Ref. 6) that extended the theory of diffusion controlled reactions with a built-in time delay. The results have application in photodissociation processes in liquid solutions.

Principal Investigators: L. Monchick, S. Green, and E. A. Mason. Dr. Monchick is a senior chemist in the Chemical Physics Group of the Research Center and will be Parsons Professor in the Chemistry Department of The Johns Hopkins University from 1 September 1975 to 1 June 1976; Dr. Green is a senior Postdoctoral Fellow at Columbia University and the NASA Institute for Space Studies, and was not funded by the program; Dr. Mason is at Brown University and was not funded by the program.

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1. L. Monchick and S. Green, "Validity of Central Field Approximations in Molecular Scattering: Low Energy CO-He Collisions," J. Chem. Phys., Vol. 63, No. 5, 1 September 1975, pp. 2000-2009.

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3. Y. S. Kim and R. G. Gordon, J. Chem. Phys., Vol. 61, 1974, p. 1.

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5. L. Monchick, "The Ehrenfest Theorem and Gas Transport Properties," Physica, Vol. 78, 1974, pp. 64-72.

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Molecular Energy Transfer

This research is directed toward an understanding of the mechanisms of molecular energy transfer in collisions of gas molecules. Types of energy involved include rotational, vibrational, and electronic. Possible transfer modes consist of vibration → translation (V-T), inter- and intra-molecular vibration → vibration (V-V), vibration → rotation → translation (V-R-T), electronic → translation (E-T), and electronic → vibration (E-V). A new area of research that has emerged involves the transfer of molecular electronic energy to microbiological systems.

Research conducted during the past year is a continuation (Refs. 1 and 2) of past investigations (Ref. 3) on the collisional deactivation of laser-excited singlet molecular oxygen $O_2(^1\Delta_g)$. The studies indicate that, although deactivation of vibration $O_2(^1\Delta_g)(v' = 1 \rightarrow 0)$ can be rapid, deactivation to the ground electronic state in most cases is quite slow. The inability of most molecules to deactivate $O_2(^1\Delta_g)$ is probably due to the fact that the transition to the ground state is doubly forbidden. However, certain molecular species such as the methylamines and ozone are distinguished by their ability to efficiently deactivate $O_2(^1\Delta_g)$. In the case of the methylamines, it has been shown that no chemical reaction occurs so the process must be physical, i.e.,

$$O_2(^1\Delta_g) + M \rightarrow O_2(^3\Sigma_g^-) + M + \text{translation}. \qquad (1)$$

For O_3, however, the possibility of chemical reaction exists since $O_2(^1\Delta_g)(v' = 1)$ represents an energy of 1.165 eV compared to the O_2-O dissociation of 1.04 eV. In this case,

$$O_2(^1\Delta_g)(v' = 1) + O_3 \rightarrow 2O_2(^3\Sigma_g^-) + O(^3P) \ . \qquad (2)$$

The quantity of experimental interest is the phase, ϕ, of the acoustic signal sensed by the microphone (see Refs. 1, 2, and 3 for details) relative to that of the exciting chopped laser beam as a function of the chopping frequency f. For the case of deactivation by the methylamines, the variation of tan ϕ with f is indicated in Fig. 1 along with that for pure O_2 (dashed curve) for comparison. Figure 2 contains a similar plot for O_2-O_3 mixtures in which O_3 concentration is varied. In both cases, the total pressure was 35 atm. The dependence of tan ϕ on f for

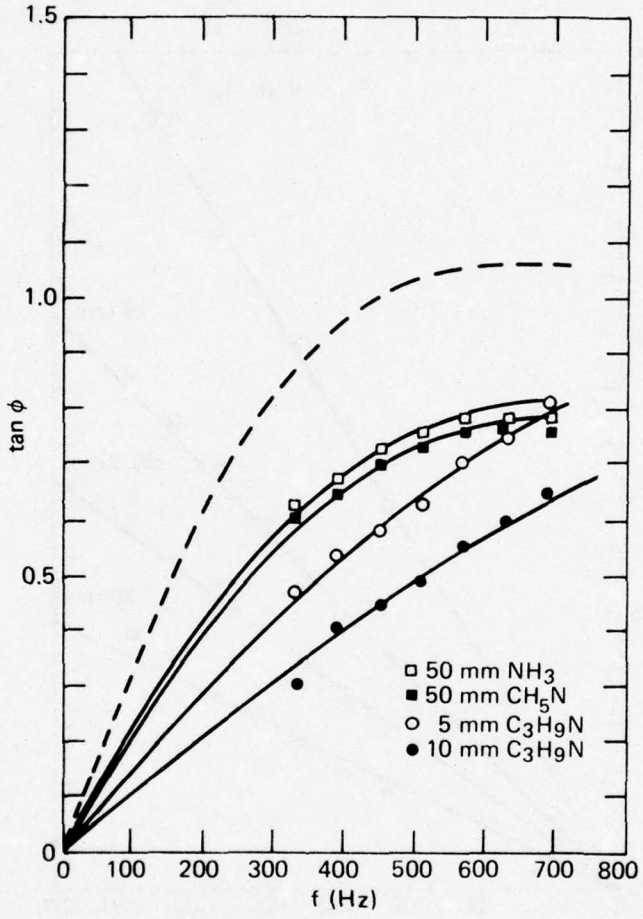

Fig. 1 Experimental Values of tan ϕ Plotted versus Frequency for O_2 Containing Trace Amounts of NH_3, CH_5N, and C_3H_9N. In all cases, the total pressure was 35 atm and the temperature 25°C. The dashed curve gives values of tan ϕ for O_2 ($^1\Delta_g$) (v′ = 0) in 35 atm O_2.

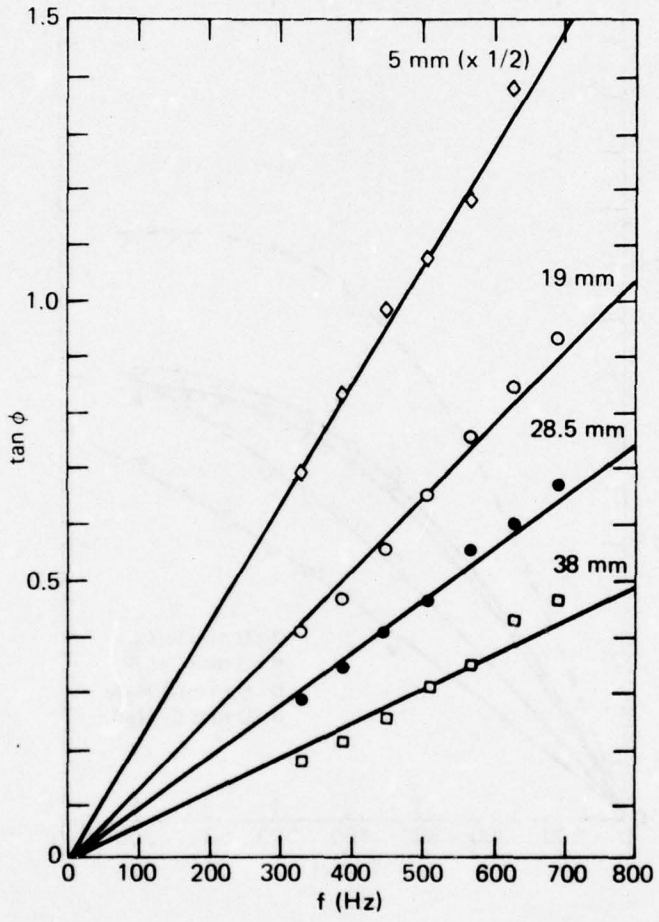

Fig. 2 Experimental Values of tan ϕ versus Frequency for Mixtures Containing Various Indicated Amounts of O_3 Pressurized to 35 atm with O_2 at a Temperature of 25°C. For the case $p(O_3)$ = 5 mm, it is necessary to multiply the plotted values of tan ϕ by a factor of two to reproduce the experimental values.

the O_2-O_3 is linear in contrast to the data for the methylamines, indicating that the deactivation by O_3 is not a simple physical process.

A possible model of the $O_2(^1\Delta_g)(v' = 1)$ deactivation by O_3 has been developed for the interpretation of the experimental data. This involves, first, the transfer of electronic energy from $O_2(^1\Delta_g)$ to form electronically excited (triplet) O_3, and then the dissociation of the latter to ground state O_2 and O. The second step appears to be the slow rate-determining process in the overall deactivation, the O formed eventually regenerating O_3 by reaction with the O_2 present in excess. The importance of these results as they affect the chemistry of the upper atmosphere — particularly the ozone layer — remains to be considered.

The second area of investigation involves the effect of laser-excited singlet molecular oxygen on microbiological systems and is based on three known results: (a) $O_2(^1\Delta_g)$ in the gas phase is known to be able to kill bacteria; (b) laser radiation of 1.06 μm can produce $O_2(^1\Delta_g)$ in mixtures of O_2 in solution with various liquids; and (c) radiation at 1.06 μm can penetrate water. Collective consideration of these three separate pieces of information suggests a means of water sterilization using a combination of oxygen pressurization with laser radiation.

A series of experiments carried out with the help of the Washington Suburban Sanitary Commission has indicated that this hypothesis is correct. Further analytical tests have established that the mode of bacteria killing involves destruction of cell walls. Moreover, it has been shown that laser radiation of the intensity used in these tests is by itself ineffective. Thus, the oxygen excited by the laser deactivates collisionally, transferring its energy to the organism to apparently a sufficient degree to cause local damage. The phenomenon of damage to biological organisms by molecular energy transfer is an interesting subject for future studies and may have significant health applications.

Principal Investigator: J. G. Parker. Dr. Parker is a senior physicist of the Chemical Physics Group of the Research Center.

References:

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MICROWAVE PHYSICS

The applications of microwave radiation in defense systems and defense oriented research are so widespread that it is essential for the Laboratory to be highly competent both in current microwave technology and in the fundamental aspects of microwave science that will be the basis for future technological applications. Furthermore, the recent advances in the generation and use of coherent infrared and visible radiation have led to a gradual broadening of the subject area beyond the pure microwave region with emphasis on areas of overlap between microwave and visible radiation.

Basic research in microwave physics and related areas has been pursued in the Research Center since shortly after its formation. The activity has provided a scientific base for dealing with a variety of new technologies including lasers, microwave optics, and microwave acoustics. In particular, the extensive military use of microwaves and other electromagnetic radiation makes it important to understand those relations between the structure of matter and its interactions with electromagnetic radiation that are important in the generation and utilization of radiation. An important byproduct of this work is the ability to carry out studies of the molecular and solid-state structure of a variety of materials with current or potential importance in defense technology. Areas where this ability has been used are: (a) the structure and chemical reactions of free radicals, a subject of importance in high energy combustion, the photochemical and oxidative decay of materials, and the synthesis of unique materials, a study that has been done in collaboration with the Electronic Physics Group; (b) the recently discovered 1-dimensionally conducting organic charge transfer salts, a study that was done in collaboration with the Quantum Electronics Group. Earlier studies in microwave spectroscopy of molecular rotational energy levels and the effects of electric and magnetic fields on these levels, electron spin resonance (ESR) studies of the so-called "color centers" in alkali halide crystals, and studies of free radicals and their reactions have made the Laboratory internationally recognized in these areas. An example of the level of experience in free radical physics and chemistry, was the major contribution of the Laboratory to the theory of the recently discovered phenomenon of chemically induced magnetic polarization in free radicals reactions, despite having no experimental program in this area. Most recently, improvements, such as techniques for growing single crystal samples, have been made in procedures for obtaining highly resolved optical spectra of complex organic molecules by incorporating them in dilute solid solutions at low

temperatures (Shpol'skii method). Molecules that can be studied in this way include laser dyes and porphyrins of importance in many areas including biology and medicine.

Dr. F. J. Adrian, Supervisor of the Microwave Physics Group, has been named Associate Editor of the Journal of Chemical Physics. During FY 75 he was invited to attend the European Chemical Society Conference on Chemically Induced Magnetic Polarization in Grenoble, France, and was awarded a travel grant from the sponsors. He was also an invited panelist at the Workshop on Microwaves as an Adjunct to Cancer Treatment of the American Association for the Advancement of Science and the National Cancer Institute held in April at the National Institutes of Health.

These studies are described in more detail in the four publications that appeared and two others that were accepted for purlication during FY 75. The Microwave Physics Group is comprised of five senior scientists, one associate engineer, and one engineering assistant.

Photoexcited Triplet Mechanism of Chemically Induced Electron Spin Polarization

The photoexcited triplet mechanism of chemically induced electron spin polarization in the photodecomposition of carbonyl compounds has been developed in detail by solving the appropriate time dependent Schrodinger equation. The prediction that the electron spin polarization depends on the orientation of a polarized photoexcitation source with respect to the external magnetic field has been observed by several groups, thereby confirming this mechanism.

Detailed knowledge of photochemical reaction mechanisms is important for such problems as detection of radiation, utilization of solar energy, photochemical degradation of materials, and syntheses of unique compounds; however, the complexity and rapidity of the elementary reactions that lead from the initial absorption of a light photon to the final product(s) make the acquisition of such knowledge very difficult. A promising technique for studying photochemical reactions utilizes the recently observed phenomenon of chemically induced magnetic polarization. This is the generic name for a number of processes involving photoexcited molecules and photolytically generated molecular fragments (free radicals) that lead to abnormal populations of the nuclear spin states of the final products and abnormal populations of the electron spin states of the free radical intermediates. The key point is that these nuclear and electron spin polarizations are sufficiently

long lived to be easily observed by nuclear magnetic resonance (NMR) and electron spin resonance (ESR), respectively, yet they result from, and thus give information about, the rapid individual steps in the photochemical reaction.

One source of chemically induced magnetic polarization, which has been analyzed extensively in previous reports, is the interplay between electron-spin-dependent chemical bonding interactions between two radicals and the nuclear-spin-dependent magnetic interactions in the individual radicals (radical pair mechanism). Although this mechanism was and is highly successful in explaining a wide variety of chemically induced magnetic polarizations, a question arose whether the radical pair mechanism or another mechanism known as the triplet mechanism was the proper explanation of the electron spin polarization observed during the photochemical decomposition of certain carbonyl compounds.

In the triplet mechanism, the electron spin polarization is initially produced in a photoexcited triplet molecule that decomposes or reacts with another molecule to give an electron-spin-polarized pair of radicals. The triplet molecule is born, so to speak, with an initial electron spin polarization because of the spin selective nature of the spin-orbit interaction (i.e., the interaction between the magnetic moment of an electron and the magnetic field resulting from its orbital motion in the electrostatic field of the molecule) that enables the molecule to make the spin-forbidden intersystem crossing (ISC) from the initially produced photoexcited singlet state into the lower energy triplet state. The resulting electron spin polarization is initially with respect to the intermolecular triplet spin states, but evolves with time into a preferential population of the electron spin states with respect to the external magnetic field.

Although attractive in many ways, the triplet mechanism was regarded with great skepticism because it required that the excited triplet react to yield the spin-polarized radical pair within 10^{-8} s or less, otherwise spin lattice relaxation, which is very effective in triplet molecules, would remove the polarization. Early experiments (carried out elsewhere) aimed at distinguishing between the triplet and radical pair mechanisms in carbonyl photolysis failed to yield clear-cut answers despite the considerable differences between the two mechanisms.

The work reported here is a detailed analysis of the triplet mechanism using a time-dependent quantum mechanical formulation to account for the rotation of the molecule during the evolution of the electron spin states. This led to several interesting conclusions, the most notable being that the electron spin

polarization depends on the relative orientation of a polarized photoexciting light and the external magnetic field (Ref. 1). Shortly after preprints of this work were sent to scientists working in the field, the predicted light polarization dependence was observed by Dr. A. J. Dobbs, and K. A. McLauchlan at Oxford University, England (Ref. 2) and Prof. J. K. S. Wan and his coworkers at Queens University, Ontario, Canada (Ref. 3), in the photochemical decomposition of various quinones. This not only confirmed the triplet mechanism as the source of the electron spin polarization in these systems but gave considerable information about the electronically excited states involved and their chemical reactivity which, as stated earlier, must be considerably faster than believed from earlier "wet chemistry" experiments. Furthermore, retention of the polarized-light-dependent initial orientation of the photoexcited singlet requires that the singlet-triplet intersystem crossing rate be comparable to the rate of molecular reorientation in solution; that is, the intersystem crossing occurs within approximately 10^{-11} s; this result agrees with picosecond spectroscopy measurements.

Principal Investigator: F. J. Adrian. Dr. Adrian is supervisor of the Microwave Physics Group of the Research Center.

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1. F. J. Adrian, "A Possible Test of the Photoexcited Triplet Mechanism of Chemically Induced Electron Spin Polarization: Dependence of the Spin Polarization on Polarized Light Orientation," J. Chem. Phys., Vol. 61, No. 11, 1 December 1974, pp. 4875-4879.

2. A. J. Dobbs and K. A. McLauchlan, "Chemically Induced Electron Spin Polarization from Photolysis with Plane Polarized Light," Chem. Phys. Ltrs., Vol. 30, No. 2, 15 January 1975, pp. 257-258.

3. B. B. Adeleke, K. Y. Choo, and J. K. S. Wan, "Chemically Induced Electron Polarization. VI. Dependence of the Spin Polarization of 1, 4-benzosemiquinone and 9, 10-anthrasemiquinone Radicals in the Orientation of the Exciting Polarized Light," J. Chem. Phys., Vol. 62, No. 9, 1 May 1975, pp. 3822-3823.

Secondary Photolysis of Alkyl Radicals

Results of the ESR investigations of the spectrum and structure of NaO_3, described in the previous report, were published during the present period (Ref. 1). Current electron spin resonance (ESR) studies of the ultraviolet photolysis of n-butyl iodide in an argon matrix at 4°K show that the products depend both on photon energy and the duration of the photolysis. The results are consistent with a secondary photodecomposition of the n-butyl radical, which is formed by the primary photolytic step of dissociating the carbon-iodine bond.

The mechanisms whereby organic molecules are decomposed by light are of importance for the photostability of various materials of importance in defense technology such as oils and plastics. They also may be important in current attempts to use photolytic methods for synthesizing useful exotic materials (Ref. 2). Despite extensive photochemical work in many laboratories, many problem areas remain. One of these problem areas is secondary photolysis; that is, the absorption of light and further photoreaction by a product of the primary photolytic step. Its occurrence is likely in those photodecomposition reactions that yield more products than can be accounted for by a single photochemical step in the reaction mechanism. Secondary photolysis is also likely to be a factor in synthetic photochemical processes using high intensity arc lamps or laser sources. A related problem is the wavelength dependence of various photochemical processes, an area that has been extremely difficult to investigate until the recent development of very high intensity arc lamps and tunable dye lasers.

For an initial study of the above phenomena, we chose the photolysis of n-butyl iodide, which should be representative of the general class of alkyl iodides whose ultraviolet photolyses lead to more products than can be explained by the expected primary process of dissociating the carbon-iodine bond. The most frequently observed additional products are hydrogen, H, atoms and methyl, CH_3, radicals. A secondary reason for choosing the n-butyl iodide photolysis was a desire to observe the electron spin resonance (ESR) spectrum of the n-butyl ($n\text{-}C_4H_9$) radical free from interfering lines of the CH_3 radical.

The study used the method of matrix isolation spectroscopy in which a dilute solid solution of n-butyl iodide in argon at 4°K was photolyzed and the free radical products subsequently examined by ESR spectroscopy. It was found that, for $\lambda > 280.0$ nm (4.44 eV), only the $n\text{-}C_4H_9$ radical was formed, but for $\lambda < 250.0$ nm (5.04 eV) H atoms and CH_3 radicals were also observed (Ref. 3).

The results for the photolysis of n-butyl iodide at 246.0 nm, including the relative growth of the various products as a function of photolysis time, are shown in Fig. 1. The n-butyl signal increases linearly and the H atom signal increases quadratically with photolysis time. The weak sharp-line CH_3 spectrum, which is superimposed on the four central lines of the n-butyl spectrum also increases supralinearly with photolysis time. These results are consistent with the photolysis mechanism involving secondary photolysis of n-butyl, as shown below.

$$C_4H_9I \xrightarrow{h\nu} C_4H_9 + I$$

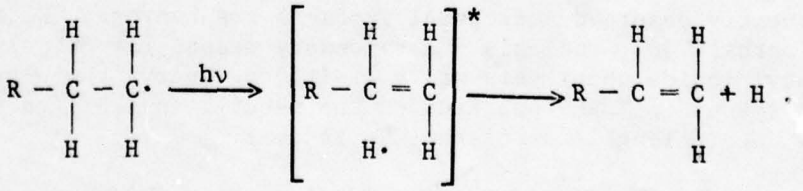
$$C_4H_9 \xrightarrow{h\nu} \begin{cases} (C_2H_5)CH{=}CH_2 + H \\ \overbrace{CH_2CH_2\dot{C}H_2} + CH_3 \ , \end{cases}$$

but not the direct photolysis mechanism

$$C_4H_9I \xrightarrow{h\nu} \begin{cases} (C_2H_5)CH{=}CH_2 + H + I \\ \overbrace{CH_2CH_2\dot{C}H_2} + CH_3 + I \ , \end{cases}$$

in which the concentrations of all products should increase linearly with photolysis time.

It is suggested that the secondary photolysis of alkyl radicals involves the photoexcitation



where the dot denotes the unpaired electron. An empirical molecular orbital calculation involving the bonding orbitals of one of the β-CH bonds and the unpaired electron orbital indicates that this transition has a sizeable oscillator strength and a lower

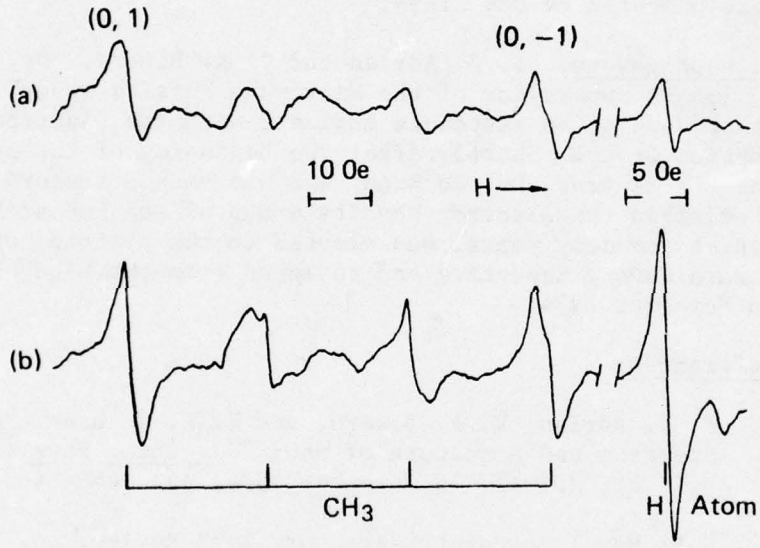


Fig. 1 Growth of Various Free Radical Species during the Photolysis at 246 nm of n-Butyl Iodide in Argon at 4°K. (a) 15-min photolysis, (b) 30-min photolysis. H atom denotes the high field hydrogen atom ESR line, and CH_3 denotes the sharp methyl lines that are superimposed on the four broader central lines of the n-butyl spectrum.

transition energy than is required for photoexcitation of the corresponding saturated hydrocarbon R-CH_2-CH_3.

Photolysis at $\lambda > 280.0$ nm instead of with a polychromatic mercury arc enabled preparation and observation of the n-C_4H_9 radical free from interference by the CH_3 radical. The resulting interpretation of the ESR spectrum clearly indicated that the two β-protons in this radical [n-$CH_3CH_2C^{(\beta)}H_2{}^{(\beta)}C^{(\alpha)}H_2{}^{(\alpha)}$] are inequivalent, a result of possible significance for understanding the interactions between nonbonded atoms that determine this secondary structural feature of the radical (Ref. 3). An earlier study of this radical by others had concluded that the β hydrogens were equivalent; however, certain critical lines of their spectrum were obscured by CH_3 lines.

Principal Investigators: F. J. Adrian and V. A. Bowers. Dr. Adrian is supervisor of the Microwave Physics Group. Mr. Bowers is an associate engineer with the Electron Physics Group. Shortly after the beginning of the present fiscal year, Dr. Cochran, who has been a senior chemist in the Electron Physics Group of the Research Center for many years, was elected to the position of Howard County Executive and resigned from the Laboratory in November 1974.

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1. F. J. Adrian, V. A. Bowers, and E. L. Cochran, "ESR Spectrum and Structure of NaO_3," J. Chem. Phys., Vol. 61, No. 12, 15 December 1974, pp. 5463-5465.

2. U.S. Naval Research Laboratory 1973 Review, pp. 99-100.

3. F. J. Adrian, E. L. Cochran, and V. A. Bowers, "ESR Study of the Photolysis of n-butyl Iodide: Secondary Photolysis and Structure of the n-butyl Radical," J. Chem. Phys., Vol. 63, No. 2, 15 July 1975, pp. 919-923.

Spectroscopic Studies of Electron Donor-Acceptor Molecules

The electronic and vibrational structure of electron donor-acceptor molecules is studied by the techniques of optical spectroscopy and electron spin resonance. The present work is concerned primarily with porphyrin molecules whose electron

transfer properties are important in biological chemical systems. The goal of this work is to correlate electronic and vibrational structure to the electron transfer properties of these molecules.

Organic molecules are becoming increasingly likely candidates for various applications; organic dye molecules, for example, are being used as laser materials. Our present studies are primarily concerned with the porphyrins that have many of the properties (optical, photoconductive, semiconductive, photochemical, etc.) deemed important. These porphyrins also have the features that make them good model compounds for studying the relation between structure and the significant properties of highly conjugated molecules. Many of the techniques being used to study porphyrins can be applied to other organics such as dye laser molecules.

High resolution absorption spectra of several metalloporphins have been first reported by this Laboratory. The sharp line spectra were obtained by a novel technique in which the metallo-porphins are incorporated as guest molecules in a single crystal organic host (triphenylene), and their spectra observed at low temperatures. The single-crystal host technique, like the previously used Shpol'skii method of incorporating the molecule under study in a glassy solid solution, greatly reduces the inhomogeneous line broadening that is responsible for the broadband spectra of organic molecules observed in solution at room temperature. However, the single-crystal method gives better resolution than the Shpol'skii method and also provides oriented guest porphin molecules that allow the polarization of the spectral transitions to be observed.

Apparatus for fluorescence spectra spectroscopy has been assembled, and some preliminary fluorescence spectra of porphyrins have been observed. In this technique one observes the emission spectrum resulting from excitation of a single sharp absorption line (our excitation source is a tunable dye laser pumped by an ultraviolet nitrogen laser). This method has several powerful advantages: (a) related lines, such as various vibrational states of the same electronic transition can be identified by their common fluorescent response, (b) the fluorescence can be time resolved, which gives information about rates of decay of different excited states, rates of energy transfer, etc., and (c) slightly different spectra resulting from the same molecule in different sites of the host crystal can be distinguished. The last point is of special importance in the porphyrin studies because the one disadvantage of the single-crystal-host technique is complication of the spectra by the presence of inequivalent sites in the host crystal.

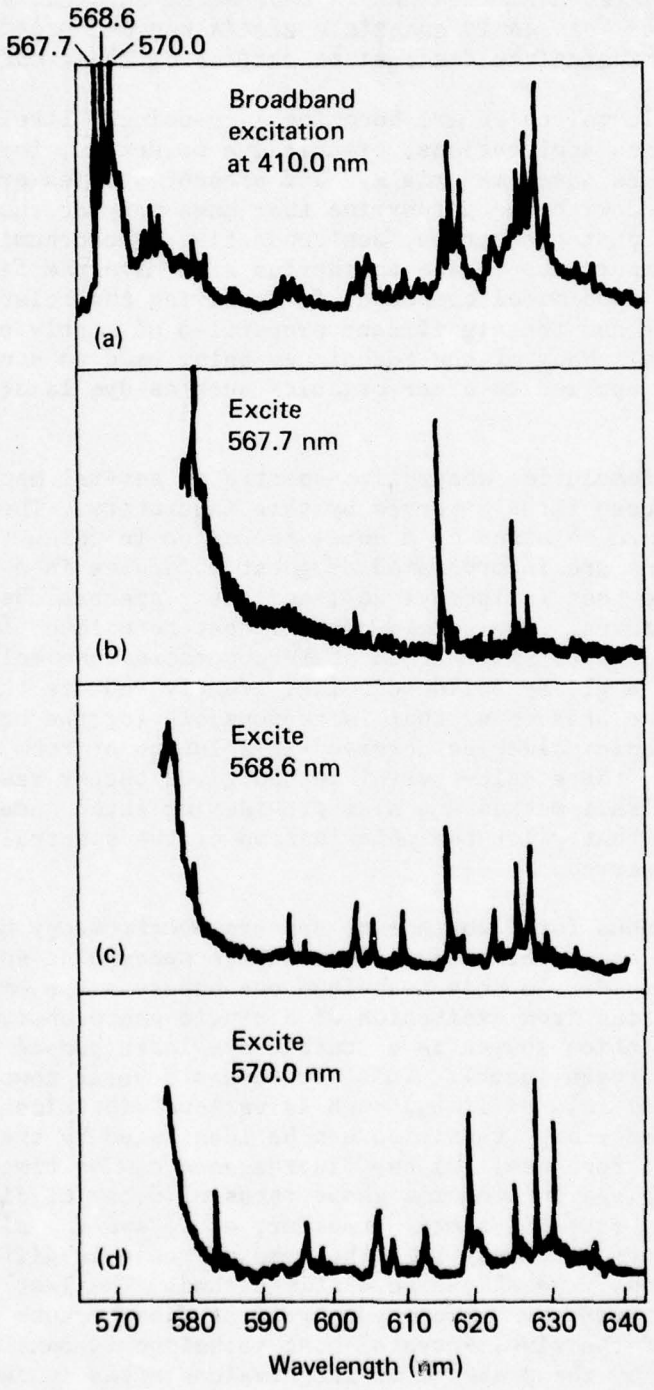

Fig. 1 Fluorescence Spectrum of Zn Porphin in Tirphenylene at 4.2° K

Preliminary spectra of Zn porphin in triphenylene have been obtained. These results, illustrated in Fig. 1, show that there are three principal sites of Zn porphin in triphenylene. The lowest excited singlet transition for each of these site species occurs at 567.7, 568.6, and 570.0 nm, respectively. Figures 1b, 1c, and 1d show the fluorescence spectrum obtained by separately exciting each of these wavelengths. In each case, these spectra originate from a single species of site. Figure 1a shows the fluorescence spectrum obtained using the conventional technique of broadband excitation. A comparison of this spectrum with the single-site spectra shows that this spectrum contains the spectra from all the principal site species. Further studies of Zn porphin and free base porphin in triphenylene are in progress using these site selection techniques.

Results on Pd porphin, Ni porphin, and free-base porphin are published in previous and current publications (Refs. 1 and 2).

Principal Investigators: B. F. Kim and J. Bohandy. Drs. Kim and Bohandy are senior physicists of the Microwave Electronics Group of the Research Center.

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Electron Transfer Luminescence in Solution

The possibility of dye laser pumping using electrochemical reactions at an active electrode as the pumping source is now under investigation. The potential utility of simultaneous electron spin resonance and optical spectroscopic experiments in clarifying the major questions of the efficiency of these reactions is discussed, and progress toward applying these methods in certain potentially useful reactions is described.

A search for more efficient excitation mechanisms for dye lasers as alternatives to optical pumping has led to renewed interest in chemiluminescent reactions. A particular subclass of

reactions of this type are those termed electrochemiluminescent and are characterized by having the process initiated by formation of reactive species at active electrodes in an electrochemical cell. The detailed mechanisms are largely unknown. Nevertheless, total electrical-to-light conversion efficiencies of 2% have been reported, and a clearer understanding of the underlying physics may permit improvements in these reported efficiencies.

Whether or not reactions produce significant light emission is related in some cases to the nonradiating character of the molecular states involved and in others to the relative efficiencies of competing nonradiative processes. The particular type of luminescent reaction selected for study is the so-called charge transfer reaction involving molecular radical ions in aprotic solvents, i.e., solvents lacking detachable hydrogen atoms. The radical ions may be formed chemically as the result of a secondary process, or electrochemically at active electrodes in electrochemical cells. The ions may be of either charge and commonly are formed by addition or subtraction of one or more electrons from a stable neutral molecule such as anthracene, naphtalene, or an organic dye such as rhodamine.

It is the objective of this project to elucidate these questions experimentally using simultaneous electron spin resonance (ESR) and optical spectroscopy. This will be combined with in situ radical ion generation in an electrochemical cell. Each spectroscopic method has been used in the past in a variety of similar problems. For example, ESR has been used to uniquely specify both kinds of radical ions present and their concentrations, and optical emission spectroscopy has been used to be similarly specific with respect to the final species responsible for light emission. It is hoped the combined information from the ESR and optical measurements will define more clearly the mechanisms of luminescence in these systems.

The initial phase of adapting a spectrometer system, used previously for optical detection of microwave absorption in solid samples, to ESR, optical spectroscopy, and possibly microwave-optical double-resonance spectroscopy on molecular ions in aprotic solvents is essentially completed. Several electrochemical cells compatible with ESR/optical detection have been designed. Preliminary ESR measurements of chemically generated radical ions have been made. A representative spectrum appears in Fig. 1. Visible emission from a simple electrochemical cell has been observed. The combined ESR/optical/electrochemical cell experiment should be ready shortly. A short paper describing instrumentation designed for this application has already appeared (Ref. 1).

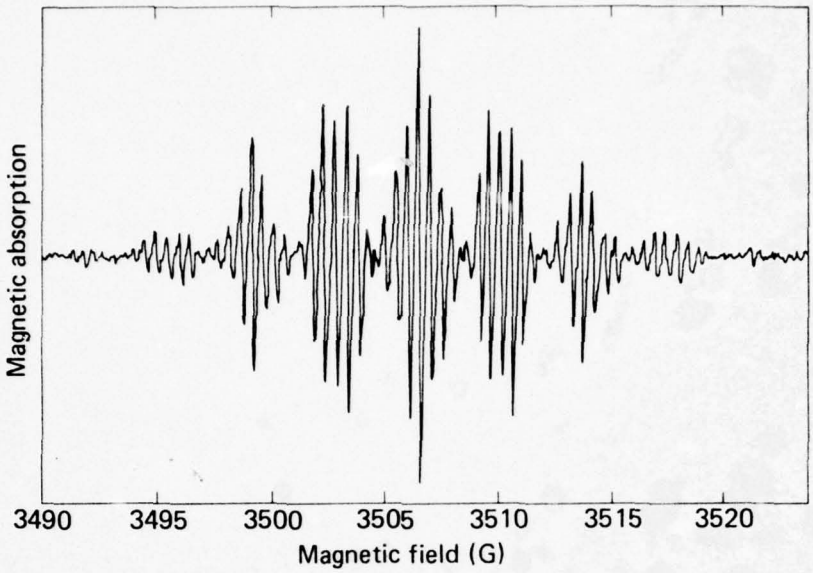

Fig. 1 Magnetic Resonance Spectrum of the Perylene Positive Ion in Concentrated Sulfuric Acid.

Simultaneous ESR and optical emission spectroscopy on chemiluminescent reactions should provide a significant new tool for the investigation of these reactions.

Principal Investigators: J. C. Murphy and L. C. Aamodt. Drs. Murphy and Aamodt are senior physicists of the Microwave Physics Group of the Research Center.

Reference:

1. J. C. Murphy, P. R. Zarriello, L. C. Aamodt, and H. A. Kues, "A Convenient ESR/ODMR Spectrometer," Review of Scientific Instruments (accepted for publication).

QUANTUM ELECTRONICS AND EXCITATION MECHANISMS

Shortly after the reported discovery of the laser, the Research Center established a group to explore the kinetic mechanisms generally associated with lasers, both from a fundamental and an applied point of view. Early basic contributions were made in He-Ne laser physics and, more recently, in the physics and chemistry of infrared lasers. Definitive contributions have been made in chemical lasers (APL was the first to demonstrate a one-atmosphere DF-CO_2 pulsed-chemical laser and to devise a chemical laser using a safe fuel-oxidizer) and far-infrared lasers useful for plasma diagnostics. Research in quantum electronics has expanded to include synthesis and analysis of newly-discovered organic conductors.

Quantum electronics per se is a rather inclusive title generally applied to the study of the interaction of radiation with matter. Lasers are a specific example, and these devices are continuing to play an important role in both military and civilian technology. Laboratory missions require familiarity with laser technology, and two Research Center Groups (Quantum Electronics and Excitation Mechanisms) are actively engaged in fundamental studies in this area. The direction of research is influenced by DoD's interest in high-energy lasers and laser radar; to this end, previously initiated investigations in chemical lasers have continued with studies of high-pressure pulsed DF-CO_2 chemical transfer waveguide lasers and in kinetic mechanisms of the safe-fueled Na-catalyzed N_2O-CO combustion laser. Additionally, the usefulness of far-infrared lasers as diagnostic tools to study thermonuclear plasmas has prompted further studies of the dynamics and lasing mechanisms of the 95 and 217 μm wavelength infrared lasing emission of the He atom.

An evolving role of the Research Center in collaboration with the Department of Chemistry of The Johns Hopkins University, has been in assessing the potential of the new class of organic conducting materials, which are of potential significance to DoD in many electrical and electronic applications. In this program organic donor-acceptor complexes are synthesized under controlled conditions, and an extensive series of physical measurements are directed toward understanding the physics of these unique materials. To date, these procedures have led to markedly increased conductivity of the first organic material (TTF-TCNQ) and the development of a new material (HMTSF-TCNQ) that exhibits high conductivity over an extended temperature range (1 to 300°K).

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Infrared Lasers: Far-Infrared Helium Laser Studies

Diagnostic studies have been made of an electrical-discharge far-infrared helium laser. Accurate wavelength measurements of 216.13 ± 0.01 and 95.763 ± 0.006 μm of laser emission have provided further verification of the previously-assigned $3^1P_1 \rightarrow 3^1D_2$ and $4^1P_1 \rightarrow 4^1D_2$ energy-level transitions. Optical probes have been used to study the spatial and temporal variation of electrons and metastable species in the plasma. These later measurements have demonstrated (a) that wall-generated electrons migrate toward the axis where their concentration is always at a minimum and (b) that quenching of laser action is due to kinetic heating that occurs during the excitation pulse. An attempt is being made to improve diagnostics of far-infrared lasers by developing a time domain microwave spectrometer.

Far-infrared lasers are important tools for thermonuclear plasma diagnostics and solid-state studies. They also have potential as precision radars if efficient high-power sources can be developed. The present studies have emphasized electrical-discharge excited He, HCN, and H_2O far-infrared lasers.

Far-infrared laser emission at 95 and 216 μm wavelength from electrical-discharge in helium have been observed in experiments conducted at APL and other laboratories. These transitions have been tentatively assigned to the transfer between the energy levels $3^1P_1 \rightarrow 3^1D_2$ (95 μm) and $4^1P_1 \rightarrow 4^1D_2$ (216 μm). If these are the appropriate upper laser level energy states, it is quite likely that inversions exist at even higher energy levels that would afford the potential of lasing action at longer wavelengths. If the energy level assignments are to be made on spectroscopically-measured wavelengths alone (as they have been), the measurements must be highly accurate. Experiments of this type were completed at APL along with basic investigations into the dynamics of the electrically-discharged helium plasma leading to lasing action. These later experiments elucidate the excitation mechanisms and the cause for the quenching of lasing action that occurs during excitation.

The operation of the helium laser is highly transient, and its output depends critically on the plasma conditions existing during emission. For example, it is found that lasing action is quenched while the discharge current is still rising even though the excitation cross sections and indicated life-times are greater for the ^1P states than the ^1D states. In the type of discharge used for our experiments, we have shown experimentally that the electrons are created at the wall and move toward the axis, producing a time-varying radial electron density distribution

with a minimum on axis that persists throughout the laser emission. The radial distribution has been studied by observing the spatial and temporal variation of the visible lines by probing the plasma with 337 μm radiation and by observing the effect of metastable atoms in the discharge on 0.5015 and 0.3965 μm radiation transmitted through the discharge. There is also a rapid increase in kinetic temperature during laser emission because of the excitation pulse; this in turn is found to increase collision frequency and prevent the inversion necessary for lasing from being maintained even for the duration of the excitation pulse (Ref. 1).

Wavelength measurements of the $3^1P_1 \rightarrow 3^1D_2$ and $4^1P_1 \rightarrow 4^1D_2$ laser transitions have been made with a far-infrared Fabry-Perot interferometer, and have yielded measured vacuum wavelengths of 216.13 ± 0.01 μm and 95.763 ± 0.006 μm (values derived from other optical measurements are 216.18 and 95.785 μm). The intensities of the visible lines associated with the upper and lower lasing states were found to correlate properly with the presence or absence of far-infrared lasing action, confirming the identity of the lasing transitions.

An improved experimental technique is being attempted through the development of a K-band time domain microwave spectrometer using a Fabry-Perot resonator for measuring the time dependence of the excitation of various gas molecules of interest as infrared laser sources. A time domain emission technique is used to measure energy relaxation times, which are the Fourier transform of pressure and wall collision broadened linewidth independent of doppler broadening. The flexible resonator configuration yields sensitivities comparable to waveguide spectrometers with various gas cells suitable for collision studies or IR double-resonance experiments (Ref. 2).

Principal Investigators: R. Turner and T. O. Poehler. Mr. Turner is a senior engineer of the Quantum Electronics Group and Dr. Poehler is the Group Supervisor.

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1. R. Turner and R. A. Murphy, "The Far Infrared Helium Laser," paper presented at International Conference on Infrared Physics, Zurich, Switzerland, August 1975 (to be published in Infrared Physics, 1975.

2. R. M. Somers, T. O. Poehler, and P. E. Wagner, "Microwave Time Domain Fabry-Perot Emission Spectrometer," Rev. Sci. Inst., Vol. 46, No. 6, June 1975, pp. 719-725.

Chemical Lasers: High-Pressure Pulsed DF and DF-CO_2 Chemical Lasers

Rapid electrical initiation of combustible D_2-F_2-He mixtures with and without CO_2 in a laser cavity has been used to study kinetic mechanisms of the DF and DF-CO_2 transfer chemical lasers at high pressure. Time-resolved emission spectra of the DF-CO_2 laser exhibits prompt laser emission from both DF and CO_2 in addition to the usual more energetic but delayed CO_2 laser emission. Studies of the time correlation of the vib-rot transitions provide evidence that the high rate of energy transfer from DF($v \leq 4$) to CO_2 involves collisional energy transfers in which the rotational level change in DF exceeds unity. Further, the delayed emission from CO_2 is mainly due to energy transferred from DF($v \leq 4$). The results provide additional valuable insight into the kinetic mechanisms of chemical lasers.

Chemical lasers are particularly attractive candidates for high-power laser systems because of the reduced requirement for auxiliary power. Chemically-pumped DF-CO_2 and DF lasers are especially attractive for military applications because the laser outputs correspond to atmospheric windows, and the Research Center has had a continuing experimental study in high-pressure pulsed DF and DF-CO_2 chemical lasers supported in part by NAVSEA. One of the early developments in this NAVSEA-supported project was the first demonstration of a pulsed DF-CO_2 chemical-transfer laser operated at pressures to 1 atm; more recently, this project led to the adaptation of this technology to a waveguide laser configuration (Ref. 1).

During the course of this research, in which very fast electrical discharges through Rogovsky electrodes were used to initiate high-pressure (ca 300-760 Torr) mixtures of He-D_2-F_2 with and without CO_2, some anomalies in the temporal laser emission were observed. Specifically, combustible D_2 + F_2 (+He + CO_2) mixtures when ignited by 150 ns electrical discharge exhibited a prompt laser radiation from the DF molecule (3.6 μm) and the CO_2 molecule (10.6 μm) followed by a delayed 10.6 μm laser pulse normally observed with slower electrical excitation pulses (450 ns or longer) or with flash photolysis initiation. This behavior is intimately related to the not-well-explained energy transfer processes in DF chemical lasers. It was felt that measurements of the time-resolved spectral output could more clearly define the excitation mechanisms. Consequently, an in-depth study of their phenomena was undertaken in the Research Center in support of the NAVSEA-sponsored program (Ref. 2). The results of that study are summarized below.

The use of fast electrical initiation makes it possible to produce electron energies (1.5 eV) near the maximum cross section for the $F_2 + e \rightarrow F^- + F$ reaction. The increased F^- concentration results in a rapid increase of excited DF from the "cold reaction," $F + D_2 \rightarrow DF^* + D$, which populates the $v = 3$ vibrational levels. The sequence of emission lines when CO_2 is present and when it is not present make it possible to demonstrate that the high rate of energy transfer from excited DF to CO_2 can be explained if the energy difference is taken up by ΔJ changes in DF of +2 or +3 as proposed by others. The main energy transfer to CO_2 is most likely due to the "hot reaction," $D_2 + F \rightarrow DF^* + D$, which populates the $v \leq 8$ states. In this case, the difference in the reaction rates for the two branches makes it possible to achieve an inversion at $v = 5$, and the energy is transferred with a $\Delta J = +1$. There is evidence in this laser that, with fast electrical excitation, an inversion can be achieved in CO_2 by direct electrical excitation of DF.

Principal Investigators: R. Turner and T. O. Poehler. Mr. Turner is a senior engineer of the Quantum Electronics Group and Dr. Poehler is the Group Supervisor.

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1. T. O. Poehler, R. E. Walker, and J. W. Leight, "High-Pressure Chemical Waveguide Laser," Appl. Phys. Ltrs., Vol. 26, No. 10, 15 May 1975, pp. 560-561.

2. R. Turner and T. O. Poehler, "Electrically Initiated Pulsed Chemical DF-CO_2 and DF Lasers," presented in part at the 4th Conference on Chemical and Molecular Lasers held in St. Louis, MO., 21-23 October 1974. The final paper was submitted for publication to J. Appl. Phys. (Abstract published in IEEE J. Quantum Electronics, Vol. QE-11, No. 8, August 1975).

Chemical Lasers: Modeling of the Na-CO Electronic-Vibrational Energy Transfer

The quenching of electronically-excited atoms by molecular species is an important if not dominant process in some laser systems. A case in point is the quenching of chemically-produced excited Na atoms by CO in the N_2O-CO chemical laser in which the Na atom is used as a catalytic agent. The problem has been examined analytically to show that energy transfer from electronically excited $Na(3^2P)$ to $CO(v = 8)$ is indeed fast, but that the

filtering of this energy into the lower vibrational levels where it is available for lasing action is slow at the pressures and temperatures of interest. The result explains in part the absence of lasing action for conditions where CO is present in excess.

Electronic-vibrational (E-V) energy transfer processes are of increasing interest recently since they are extremely fast (essentially gas kinetic in many cases) mechanisms for the deactivation of excited states involved in visible lasers. E-V processes also provide a potential means of achieving lasing in the visible region via rapid energy transfer from vibrational levels to excited electronic levels. In addition to providing a basic understanding of E-V transfer, processes involving sodium atoms are of immediate interest with regard to the pumping mechanism of the Na-catalyzed N_2O + CO chemical laser developed at APL (Ref. 1). The present work provides basic understanding that complements directly funded (NAVSEA) work on the CW chemical laser.

One of the proposed mechanisms of the N_2O chemical laser involves the direct production of electronically excited sodium, $Na(3^2P)$, in the chemical reaction:

$$Na + N_2O \rightarrow NaO + N_2 + 21.0 \text{ kcal/mole}$$

$$NaO + CO \rightarrow CO_2 + Na(3^2P) + 17.6 \text{ kcal/mole.}$$

The $Na(3^2P)$ energy is then rapidly transferred to the vibrational levels of N_2, CO, N_2O, and CO_2. Since there is rapid V-V transfer between the vibrational levels of all four molecules, equilibrium is readily established between the asymmetric stretch modes (upper laser levels) of CO_2 and N_2O and the vibrational levels of CO and N_2. Because of this equilibrium and energy sharing, when N_2O is the major constituent, most of the energy is deposited in the N_2O vibrational levels. This results in the N_2O species lasing at 10.8 μm.

However, when N_2O is a minor constituent and there is a large excess of CO, no lasing at 10 μm has been observed. A possible explanation is that most of the energy will be transferred to the CO(v) levels, presumably those levels that are most resonant with $Na(3^2P)$, i.e., CO(v = 7,8,9). Since it is known that the V-V relaxation of CO by CO itself is rather slow for the high vibrational levels, then the energy might remain trapped in CO(v).

In order to obtain an estimate of the time evolution for the CO(v) population during the E-V transfer from $Na(3^2P)$, a system of differential equations describing the rate processes was solved using standard computer techniques. The rate constants and radiative lifetimes of all the pertinent levels have been previously measured. However, it is not known which CO vibrational level is most important in the transfer. Thus the calculations were simplified by constraining the E-V process to involve only $CO(v = 8)$, the level most nearly resonant with $Na(3^2P)$.

The results for typical pressures of $P_{Na} = 0.02$ Torr and $P_{CO} = 2.0$ Torr and initial electronic temperatures of sodium $T_e = 1500$, 2000, and 2500°K all show that the E-V transfer to $CO(v = 8)$ is essentially complete in 10^{-7} s and that the CO(v) levels for $v > 4$ remain highly populated, i.e., equilibrium among CO(v) is not established even after 1 ms. This is rather long relative to most energy transfer times and may explain why no lasing has been observed from CO_2 or N_2O when CO is the major constituent. Experiments are in progress to measure the gain (or loss) for CO(v) in the $Na\text{-}N_2O + CO$ system and thereby determine if the upper vibrational levels of CO are indeed highly populated because of the efficient E-V transfer from Na.

Principal Investigator: R. C. Benson. Dr. Benson is a senior chemist in the Excitation Mechanisms Group.

Reference:

1. R. C. Benson, C. B. Bargeron, and R. E. Walker, "Gain Measurements in a Transverse-Flowing $Na\text{-}N_2O + CO$ Chemical Laser," Chem. Phys. Ltrs., Vol. 35, No. 2, 1 September 1975, pp. 161-166. See also D. J. Benard, R. C. Benson, and R. E. Walker, "N_2O Pure Chemical CW Flame Laser," Appl. Phys. Ltrs., Vol. 23, No. 2, 15 July 1973, pp. 82-84.

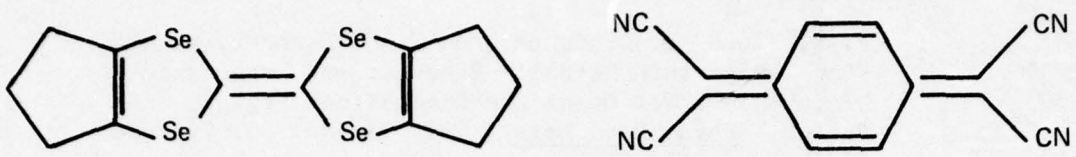
Organic Conductors

Development of new organic conductors of exceptional conductivity, and chemical control of their electronic properties is in progress in collaboration with the Department of Chemistry of The Johns Hopkins University. A steady progression has been achieved from the original development of TTF-TCNQ, which raised the electronic conductivity of the organic metallic states by orders of magnitude, to the recently synthesized HMTSF-TCNQ, which extends the range of metallic conductivity from 300°K to at least 1°K.

The first organic material to behave electrically as a metal throughout the temperature range 1 to 300°K is the compound hexamethylene-tetraselenafulvalenium tetracyanoquino-demathanide (HMTSF-TCNQ), which was developed and studied during the present year (Ref. 1). The molecular structure of HMTSF-TCNQ is illustrated in Fig. 1. The donor molecule is the logical extension of the tetramethyl analogs TMTTF (Ref. 2) and TMTSF (Ref. 3), which become insulating at low temperatures. The room temperature DC conductivity of HMTSF-TCNQ of over 2000 $(\Omega cm)^{-1}$ is the largest of any known organic substance. However, in contrast to other one-dimensional organic conductors that undergo transitions from metallic to insulating phases as the temperature is lowered, HMTSF-TCNQ remains metallic to below 1°K. Preliminary X-ray crystal structure studies show this compound to be the most nearly two-dimensional conductor of the TTF-TCNQ family. The low-temperature metallic behavior may arise from the two-dimensional suppression of the Peierls instability as well as the lack of long-range order along the weakly coupled *a* axis of the crystal.

The difficulties inherent in the conventional four-probe DC conductivity measurements in highly anisotropic crystals are avoided by use of microwave techniques. Microwave conductivity measurements of organic conductors were first made at APL, and the early measurements of TTF-TCNQ were in substantial agreement with previously obtained DC results (Ref. 3). More recently, these techniques were applied to HMTSF-TCNQ with the results shown in Fig. 2. These studies have now been extended to theoretical and experimental studies of the microwave response of small, strongly anisotropic conductors. The results have been used in properly interpreting measurements of conductivity and dielectric constant in samples of TTF-TCNQ of varying chemical purity to evaluate critically the relative importance of crystal perfection and chemical purity in determing the sample-dependent electrical parameters of TTF-TCNQ (Ref. 4). Results of general applicability have been obtained, allowing proper interpretation of microwave loss and electron spin resonance experiments over a wide range of experimental parameters (Ref. 5).

Principal Investigators: T. O. Poehler, D. O. Cowan, and A. N. Bloch. Dr. Poehler is Supervisor of the Quantum Electronics Group of the Research Center. Dr. Cowan is Professor of Chemistry and Dr. Bloch is Associate Professor of Chemistry at The Johns Hopkins University, and are not supported by the IR&D Program.



(a) HMTSF

(b) TCNQ

Fig. 1 Molecular Structure of HMTSF and TCNQ

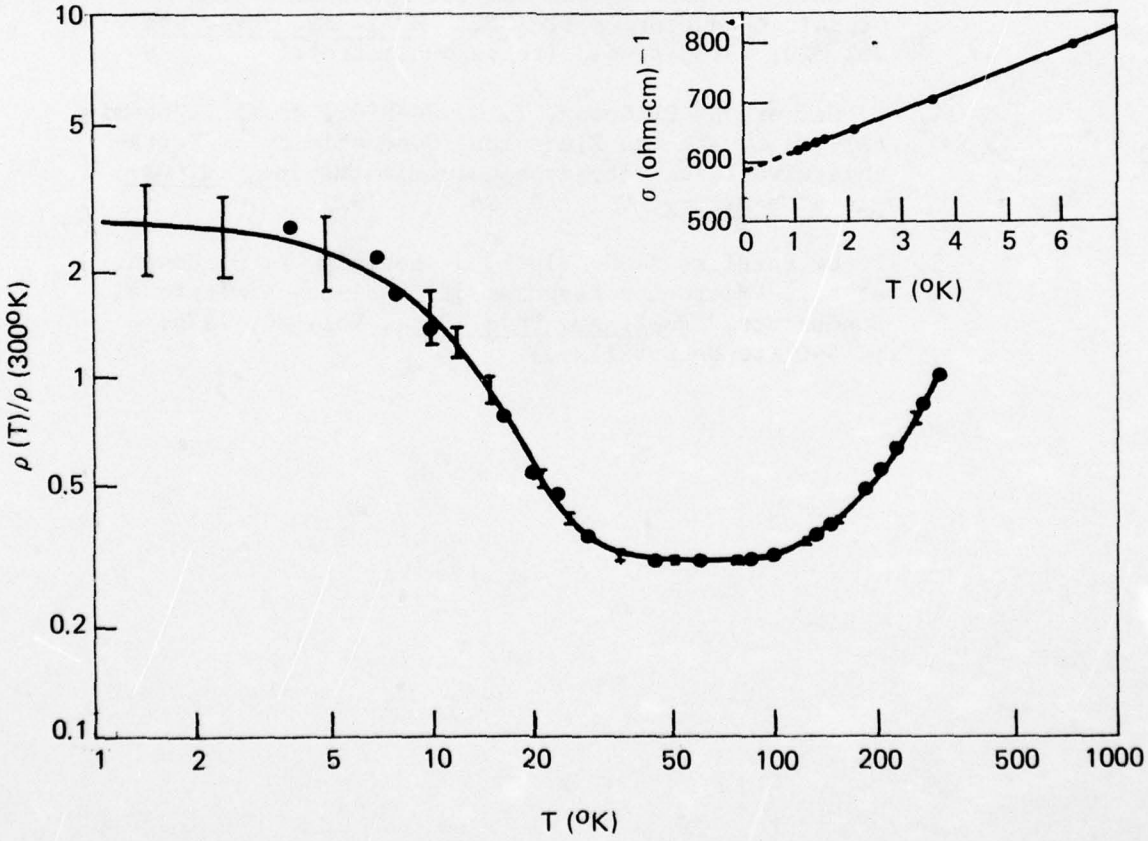


Fig. 2 Normalized DC (solid line) and Microwave (•) Resistivities of HMTSF-TCNQ (nine samples). Inset: DC Conductivity of Typical Crystal near T = O.

References:

1. A. N. Bloch, D. O. Cowan, and T. O. Poehler, et al., "Low Temperature Metallic Behavior and Resistance Minimum in a New Quasi-One-Dimensional Organic Conductor," Phys. Rev. Ltrs., Vol. 34, No. 25, 23 June 1974, pp. 1561-1564.

2. T. J. Kistenmacher, T. E. Phillips, D. O. Cowan, A. N. Bloch, and T. O. Poehler, "Crystal Structure and Diffuse X-Ray Scattering in the 1.3:2 Salt of 4,4',5,5'-Tetramethyl-$\Delta^{2\cdot 2'}$-bis-1,3-Dithiole (TMTTF) and 7,7,8,-Tetracyano-p-quinodinethane (TCNQ), a Non-Stoichiometric Quasi-One-Dimensional Organic Conductor," Acta Crystallographica (in press).

3. R. E. Pyle, A. N. Bloch, D. O. Cowan, T. O. Poehler, et al., "Conducting and Insulating Forms of the New Organic Conductor TMTSF-TCNQ," Bull. Am. Phys. Soc., Vol. 20, 1975, p. 415 (to be published).

4. R. Gemmer, D. O. Cowan, T. O. Poehler, et al., "Chemical Purity and the Electrical Conductivity of Tetrathiafulvalinium Tetracyanoquinodimethanide," J. Organic Chemistry, Vol. 40, No. 24, 1975.

5. T. O. Poehler, A. N. Block, J. Bohandy, D. O. Cowan, et al., "Microwave Response of Quasi-One-Dimensional Conductors," Bull. Am. Phys. Soc., Vol. 20, 1975, p. 440 (to be published).

SOLID STATE PHYSICS

The Solid State Physics component of the Research Center's IR&D program continues to be oriented towards providing an innovative capability in newly developing areas, primarily of inorganic amorphous semiconductors, through research in the development and application of new concepts and techniques. (Other aspects of solid-state physics are carried on in other IR&D projects summarized elsewhere in this report.)

Emphasis continues to be placed on amorphous semiconductors which have been the subject of considerable investigation in recent years both at the Laboratory and elsewhere. Substantial contributions continue to be made and internationally recognized; during the present period Dr. K. Moorjani, the group's theoretical physicist, spent most of the year in France, having been appointed by the French govenment to a visiting professorship at the University of Grenoble and a concurrent term at the Phase Transition Laboratory of the National Center for Scientific Research at Grenoble. The Group's work is described in detail in two cited reports, in three publications that appeared in print during the current year, and in five papers that have been accepted for publication. Specific projects undertaken in FY 1975 are as follows:

1. Switching in amorphous boron films;
2. Effects of carbon and hydrogen impurities in amorphous boron;
3. Mössbauer effects in solids;
4. Kinetics of amorphous to crystalline transformation in germanium films;
5. Sputtering processes in sputter-ion source mass spectrometry;
6. Thin-film crystalline silicon solar cells; and
7. Theory of disordered solids.

These interrelated projects are described briefly below.

Switching in Amorphous Boron Films

Steady-state and pulse-switching-time studies in amorphous boron, boron plus carbon, and silicon thin films show the

presence of filament formation and relate transition times to RC time constants. At low frequencies, recovery time is proportional to power dissipated in the filament; delay time is inversely proportional to sample thickness. New results for short pulses are obtained, and a previously proposed model is refined.

Switching in elemental amorphous semiconductors and chalcogenide glasses is of considerable interest, partly because of potential applications to well-known electromagnetic pulse protection problems. In this connection, a substantial part of the Research Center's switching studies have been supported by the Army's Harry Diamond Laboratories. During the present period, measurements of switching times have been extended into the nanosecond region, and phenomena associated with pulsed high-voltage signals examined. The previously developed model combining both the thermal and the electronic switching processes (Ref. 1) has been refined. Details of time dynamics in the instability process in boron is described further in Ref. 2. It has been determined that phenomena at voltages higher than those required for switching are in keeping with the electrothermal model; a paper reporting these new results is being submitted for publication.

Principal Investigators: C. Feldman, H. K. Charles, Jr., and G. Turner. Dr. Feldman is Supervisor of the Solid State Group of the Research Center; Dr. Charles, Jr. is a senior engineer of the Microelectronics Group of the Engineering Facilities Division; Mr. Turner is a doctorate student at The Johns Hopkins University.

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1. H. K. Charles, Jr., and C. Feldman, "Switching Times in Amorphous Boron, Boron Plus Carbon, and Silicon Thin Films," J. Appl. Phys., Vol. 46, 1975, p. 819.

2. "A Study of Amorphous Semiconductors for Symmetrical Varistor Applications," APL Project Z730, Final Report, 12 June 1975.

Effects of Carbon and Hydrogen Impurities in Amorphous Boron

Carbon and hydrogen were placed in amorphous boron by deposition in a partial pressure of acetylene. Carbon in amorphous boron has the effect of increasing the resistivity of the film, which is opposite to the reported effect of carbon in crystalline boron. The increase of resistivity appears to be a compensation effect of carbon in boron. Hydrogen appears to reduce

the number of dangling bonds in the amorphous network. Infrared optical experiments have been performed on boron films, which quantitatively indicate the presence of carbon and hydrogen, and roughly correlate with SIMS studies of the same samples.

The possibility of developing stable, room-temperature switching devices, very high-resistance thin-film resistors, and energy barriers emerge from our investigations of carbon-doped amorphous boron. The resistivity, electron paramagnetic resonance (EPR), and Poole-Frenkel effect have been investigated in amorphous boron films containing controlled amounts of carbon and hydrogen impurities (Refs. 1 and 2). Samples were formed on fused silica substrates by the previously used electron beam deposition method at a rate of 1.5 to 2.0 nm/s. Controlled introduction of carbon (and hydrogen) was achieved by introducing acetylene and using a gas analyzer to monitor the result. Composition analysis was achieved using a sputter-ion source mass spectrometer. EPR signals, thought to arise from dangling bonds as in amorphous Si and Ge films, remained unaffected by carbon but tended to decrease with increasing hydrogen. Resistivity was found to increase by more than two orders of magnitude with increasing carbon content, indicating the possibility of developing high-resistance thin-film resistors. (The effect of carbon on switching behavior has been previously described.) Results and interpretation are described in detail in Refs. 1 and 2.

Principal Investigators: C. Feldman, F. G. Satkiewicz, H. K. Charles, Jr., and J. Bohandy. Dr. Feldman is Supervisor of the Solid State Group; Dr. Satkiewicz is a senior chemist of the Solid State Group of the Research Center. Dr. Charles, Jr. is a senior engineer of the Microelectronics Group of the Engineering Facilities Division. Dr. Bohandy is a senior physicist of the Microwave Physics Group of the Research Center.

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1. C. Feldman, H. K. Charles, Jr., F. G. Satkiewicz, and J. Bohandy, "Electrical Properties of Carbon-Doped Amorphous Boron Films," Proceedings of the Fifth International Symposium on Boron and Borides, Bordeaux, France, September 1975 (to be published).

2. C. Feldman, K. Moorjani, and N. Blum, "Mass Spectrometry, Optical Absorption, and Electrical Properties of Amorphous Boron Films," Boron — Production, Structure, and Properties, F. N. Tavadze (Ed-in-Chief), Science Publishing House, Moscow 1974, p. 130 (in Russian).

Mössbauer Studies

Investigations of the amorphous-to-crystalline phase transformations continued with Mössbauer studies on tellurium being reported at the International Conference on the Applications of the Mössbauer Effects (Ref. 1). In this work, the amorphous-to-crystalline transition produced a large change in the Mössbauer recoil-free fraction, and a small but measurable change in the quadrupole splitting of the tellurium spectrum. These results were interpreted in terms of changes in the microscopic structure of the sample going through the transformation. In addition, Mössbauer studies of hyperfine interactions were undertaken on a well-characterized sample of europium telluride and will be reported at the December meeting of the Conference on Magnetism and Magnetic Materials (Ref. 2).

It is important to understand the relation between the properties of amorphous materials and their degree of order. Mössbauer spectroscopy has been a well-known technique for studying order in crystalline materials, and its use was first extended to elemental amorphous semiconductors at this Laboratory.

Work of the current period has dealt primarily with Europium Telluride (EuTe). EuTe is the only member of the europium chalcogenides that is antiferromagnetic; there has been considerable controversy concerning the interpretation of its properties. It is a cubic antiferromagnet with a Néel temperature of 9.6°K. In conducting samples there is a spontaneous magnetic moment below T_N.

In collaboration with Dr. R. B. Frankel (Massachusetts Institute of Technology, not funded by the IR&D program) we have used the 35.5 keV Mössbauer transition in ^{125}Te to examine the nature of the hyperfine field. At 77°K, the spectrum shows a single broadened absorption line compared with nonmagnetic ZnTe, indicating the absence of significant electric quadrupole splitting. At 4.2°K the linewidth increased by a factor of 1.5, equivalent to an average hyperfine field at the Te sites of about 80 kOe, in agreement with recent nmr measurements. The line continued to broaden with increasing external longitudinal magnetic field up to 75 kOe at 4.2°K. These observations were interpreted in terms of the magnetic field/temperature phase diagram and compared with models for the Eu spin system involving canting or nonuniform spin distribution associated with impurities.

Principal Investigators: C. Feldman and N. A. Blum. Dr. Feldman is Supervisor and Dr. Blum is senior physicist of the Solid State Group of the Research Center.

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1. N. A. Blum and C. Feldman, "Mössbauer Investigations of Amorphous and Polycrystalline Tellurium," J. de Physique, Vol. C6, p. 401 (Proceedings of the International Conference on the Applications of the Mössbauer Effect, Bendor, France, 1974).

2. N. A. Blum and R. B. Frankel (MIT), "Hyperfine Interactions in Antiferromagnetic EuTe Using the ^{125}Te Mössbauer Resonance," Proceedings of the 21st Annual Conference on Magnetism and Magnetic Materials, Philadelphia, Pennsylvania, 9-12 December 1975 (to be published).

Kinetics of the Amorphous-to-Crystalline Transformation in Germanium Thin Films

The amorphous-to-crystalline transformation in vacuum-deposited germanium thin-film samples was studied by measuring the time and temperature dependence of their optical transmission. The transformation curves obtained optically were then converted to volume transformation-time curves, giving a possible measure of the degree of amorphicity within samples. The kinetics of the process are described by an equation that contains a parameter identified with the self-diffusion activation energy of the corresponding crystalline material.

In order to make effective use of semiconducting amorphous films in electronic device technology, it is necessary to understand the mechanism of transformation to the crystalline state in as much detail as possible. Through this understanding, there is the possibility of controlling the size and growth pattern of grains during the crystallization process. The work also provides important information for studying temperature-dependent properties of amorphous films without crystallizing the samples or introducing impurities.

Films of amorphous germanium prepared by vacuum deposition were subsequently heated for various times at different temperatures. Optical transmission of the films was measured at wavelengths where the absorption is most strongly affected by the change from the amorphous to the crystalline state. Isothermal transformation curves of volume transformed versus time were described by a semiempirical kinetic equation that characterized various states of the transformation. From the isothermal transformation curves, a time-versus-temperature plot of crystallization

can be prepared that is described by a simple exponential dependence of time as a function of reciprocal temperature. A detailed report of this work has been accepted for publication (Ref. 1).

Principal Investigators: C. Feldman and N. A. Blum. Dr. Feldman is Supervisor of the Solid State Group and Dr. Blum is a senior physicist of the Solid State Group of the Research Center.

Reference:

1. N. A. Blum and C. Feldman, "The Crystallization of Amorphous Germanium Films," J. Non-Crystalline Solids (to be published in 1976).

Sputter-Ion-Source Mass Spectrometry

Extensive sputter-ion-source mass spectrometer studies have been performed on samples prepared at this Laboratory as well as on Cu_2S/CdS solar cells from the University of Delaware and GaAs crystals from the Naval Research Laboratory. Studies have continued in order to obtain a detailed understanding of the mechanisms of secondary ion generation by sputtering. The solar cell investigation has identified fabrication effects and cell impurities; the investigation of sputtering mechanism has provided a method for determining detection limits for impurities under certain adverse conditions.

The sputter-ion-source mass spectrometer (SIMS) acquired last year has proved invaluable for impurity analysis and understanding the physical properties of materials. The beam of the ion source interacts with the target (sample), producing atomic and polyatomic fragments of which some fraction is ionized. These secondary ions are focused electrostatically into a double-focusing mass spectrometer.

The capability of the SIMS for obtaining depth profiles of both ionic and polyatomic constituents has been used to study various copper sulfide/cadmium sulfide (Cu_2S/CdS) solar cells to determine the effect of processing on composition profiles and presence of impurities. Differences in constituent profiles caused by processing have been observed. The results of this work are presented in the Exploratory Development Section of this report under the topic Solar Cell Research and are described in detail in Ref. 1.

Although sputter-ion-source mass spectrometers have been available for several years, the mechanism of ion generation by sputtering is still not thoroughly understood. One of the practical consequences is the need for ad hoc time-consuming empirical calibration procedures. Accordingly, studies to characterize and clarify the sputtering mechanisms have been continued. It is particularly important, for double-focusing instruments where the secondary ion energy/window is variable, to characterize the energy dependence of secondary ion distributions. Determination curves were made for several materials. This approach enables an analyst with any such instrument to determine detection limits for impurities at masses where isotope ratio measurements are not possible and when instrument resolution is insufficient to decouple interfering species. Results are described in detail in Ref. 2.

Principal Investigators: F. G. Satkiewicz and H. K. Charles, Jr. Dr. Satkiewicz is a senior chemist of the Solid State Group of the Research Center and Dr. Charles is a senior engineer of the Microelectronics Group of the Engineering Facilities Division.

References:

1. F. G. Satkiewicz and H. K. Charles, Jr., "Sputter Ion Mass Spectrometer Analysis of Copper Sulfide/Cadmium Sulfide Solar Cell Samples," APL/JHU TG 1234.

2. F. G. Satkiewicz, "Initial Energy Distributions of Secondary (+) Ions from the Sputtering of Non-Metallic Solids with Ar^+ (3 KeV to 10 KeV)," Proceedings of the 23rd Meeting of the American Society for Mass Spectrometry, Houston, Texas, May 1975 (to be published).

Thin-Film Solar Cells

Work on thin-film silicon solar cells was initiated. Techniques for depositing pure films with thicknesses greater than the required 10 μm were developed. Studies on conversion of the amorphous thin films to the crystalline phase and on doping by diffusion were conducted. Doping profile studies using SIMS were begun. Appropriate deposition masks for solar cells were fabricated.

The high cost of presently available silicon solar cells derives in large part from intricate crystal growing steps necessary to their manufacture. These expensive steps might be avoided if a way could be found to merely deposit a thin film of silicon in the disordered state, and use the amorphous-to-crystalline phase transition. The p-n junction is then formed by a diffusion process.

APL has pioneered in the development of advanced techniques for vacuum deposition of pure amorphous films, for converting these layers to the crystalline phase, and for creating p-n junctions in such layers. The present period marks the beginning of a project to extend these techniques to the formation of vacuum-deposited thin-film solar cells. The project will emphasize (a) forming cells with efficiency comparable to that obtained in single-crystal bulk material and (b) fabrication techniques that lead to low-cost cells. Substrate interactions, diffusions and impurity, and doping profiles will be studied using sputter-ion-source mass spectrometry.

Preliminary work has been encouraging. Techniques for achieving pure amorphous films of appropriate thickness ($\gtrsim$ 10 μm to ensure absorption of light) have been developed and proved to be successful. Further studies have been initiated on the amorphous-to-crystalline transition with emphasis on achieving maximum grain size (e.g., minimum number of barriers). Diffusion studies to produce p-n junctions have been initiated but, in the absence of knowledge of diffusion constants for such films, necessarily proceed empirically and slowly.

Principal Investigators: C. Feldman, F. G. Satkiewicz, and H. K. Charles, Jr. Dr. Feldman is Group Supervisor and Dr. Satkiewicz is senior chemist of the Solid State Group of the Research Center. Dr. Charles is a senior engineer of the Microelectronics Group of the Engineering Facilities Division of the Laboratory.

Theory of Properties of Disordered Solids

Relatively little theoretical work on the properties of disordered solids was continued as a part of the IR&D program, since Dr. Moorjani was on leave of absence for 11 months of the year as a visiting professor in Grenoble, an appointment funded by the French government. However, a study by him was initiated and completed, in collaboration with Dr. S. K. Ghatak (C.N.R.S. Phase Transition Laboratory, Grenoble, not funded by the program).

The work deals with site and bond disorder in a Heisenberg Ferromagnet, a disordered solid in which a fraction c of lattice sites are randomly occupied by magnetic atoms and the remaining sites are occupied by nonmagnetic atoms. Bond disorder is introduced by allowing two possible bond strengths; the magnetization and magnetic susceptibility are developed and interpreted in terms of the Bethe-Peierls-Weiss approximation. The results are being prepared for publication (Ref. 1).

Principal Investigator: K. Moorjani. Dr. Moorjani is a senior physicist of the Solid State Group of the Research Center.

Reference:

1. S. K. Ghatak (C.N.R.S., Grenoble) and K. Moorjani, "Structurally Disordered Heisenberg Ferromagnet," Solid State Communications (to be published); M. Avignon (C.N.R.S., Grenoble) and K. Moorjani, "Order Parameter Dependence of Band Splitting in C.P.A.," Bull. Am. Phys. Soc., Vol. 20, 1975, p. 412.

EXPLORATORY DEVELOPMENT

Introduction

About one-fourth to one-third of the Laboratory's indirectly funded work is generally devoted to exploratory development studies aimed primarily at advancing the definition of new concepts related to Laboratory missions. These studies nurture the growth of innovative approaches to the point of clarifying the need for their incorporation into directly funded tasks. Examples of past contributions include the Navy Satellite Navigation System, Transit; the automatic detection and tracking system, AN/SYS-1; Dual-Mode Redeye; the Box-Launcher; and electrostatic stabilization of aircraft.

In general, the IR&D Exploratory Development projects are initiated and carried out on a short-term and part-time basis by experienced principal investigators whose primary responsibilities are to directly funded Laboratory missions. Authorization for each project, including levels of effort and funding, must be obtained in advance from the Office of the Director of the Laboratory.

Although the Applied Physics Laboratory is engaged primarily in support of national defense objectives, it also engages in projects that are directly funded by civilian agencies of the government. Thus, IR&D Exploratory Development projects are carried out also in civilian-related areas. These projects enhance the transfer of defense-related science and technology to important nondefense problems by nurturing the growth of innovative approaches to clarify their potential value. Examples of past and present contributions include the development of new concepts of navigation, air traffic control, communications, urban transportation, energy utilization, and medical technology.

The Research Center has been engaged in 24 exploratory projects during the present reporting period. As in the past, these are generally short-term efforts and relatively small; most of the work was done at levels of less than one man year. Their quality and productivity derives in large part from the competence and experience of the senior investigators and relevance to larger directly-funded programs.

The exploratory projects are individually summarized (except for the very smallest) in the following parts of this section. However, those adjudged too small for individual summaries are worthy of mention.

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One very small exploratory study, extending part time over a period of four months, provided Laboratory participation in an assessment of Automated Guideway Transit Systems conducted by the Congressional Office of Technology Assessment. The results of the study were reported to the Senate Appropriations Subcommittee on Transportation (Senate Hearing, Department of Transportation and Related Agencies Appropriations, Fiscal Year 1976, 94th Congress, First Session, H.R. 8365, part 2) and have been published (Ref. 1).

A second small project (total, approximately 4 man months) is concerned with the application of new techniques to air traffic safety problems. The first objective is the application of the new technology of charge-coupled devices to video quantizers. Specific application is to solve inadequate performance problems of the analog delay line of an analog rank quantizer (built elsewhere) for the FAA en-route system. Success with the application has potential benefits in the development of any type of video quantizer. The second objective is developing a method for automated air traffic advisory service utilization of track-file data. (Currently, automated air traffic control tracking systems assess the position coordinates of reported aircraft positions relative to selected tracks for preset neighboring regions around each track. This information is used to update the current track files and then deleted, but it is also information that is provided to pilots by traffic advisory services generated by the controller.)

In a third small (1.5 man month), short-term exploratory effort, weapon system simulation studies were carried out to investigate the advantages of applying ramjet propulsion systems, such as those being developed at this Laboratory, to future antiship missiles (ASM's) and antiair missiles for antiship missile defense (ASMD) systems. Six missiles were considered in kinematic studies of various threats using, principally, appropriately extended weapons simulations previously developed and used by the Systems Analysis Group. For reasons of national security, the results of this study are classified, but have been published and are available to properly authorized individuals.

A very small (1 man month) experimental investigation, started near the end of last year and completed early in the present year, established the feasibility of using a single traveling wave tube for the radar altimeter and microwave-scatterometer in SEASAT-A .

Three other small-scale exploratory studies (total level of effort 2.1 man months) were initiated late in the present

reporting period. The first of these is an outgrowth of a real time hemodynamic monitoring unit developed in the Myocardial Infarction Research Unit Program (MIRU) with the Johns Hopkins Medical Institutions. As a result of that development, the advantages for portability became apparent. The project was initiated to investigate the design and fabricate from one to four portable monitoring units and test their utility in a variety of clinical environments. Much of the preliminary feasibility analysis has been completed, and participating physicians have been identified.

The second, very late-start exploratory effort, was initiated to support the real time generation of sophisticated tactical displays for Navy ships, using high-speed access mass-storage devices. Equipment to support this study has been identified. When the equipment is delivered, it will be interfaced and preliminary applications will be tested.

The third late-start project (0.6 man month during the present year) deals with problems of assuring equipment readiness through the development of an Automated Maintenance Support Tool (AMST) that can interact with and provide broad support to an operator during routine maintenance and diagnostic repair. The need is a result of the increase in sophistication of individual components in Combat Weapon Systems, where readiness is frequently limited by the ability to maintain equipment. Moreover, in the case of smaller ships the ability to maintain equipment with a small crew has resulted in an effective ceiling on the complexity of the components deployed. Thus, a significant increase in the ability to maintain equipment can directly result in an increase in combat effectiveness. The preliminary studies indicate that it will be possible to demonstrate an AMST with features to include:

1. Programmed support for routine maintenance and standard diagnostics for a given equipment set, and a mechanism for including additional programmed support for an arbitrary equipment set;

2. Nonprogrammed access to and display of technical data including text, drawings, waveforms, computations, etc., to support troubleshooting in situations for which no diagnosis has been anticipated; and

3. Ability to be inexpensively mass produced in a semiportable model that can directly interface with standard test equipment.

One small exploratory study (approximately 1 man month) concerned with internal combustion engines was initiated at the end of the previous period and completed during the present period. Currently, low pollutant emissions from such engines are generally achieved by operating at high fuel/air ratios (lean burn), and relying on some form of after-treatment such as a catalytic converter. Primary limiting factors are cycle-by-cycle variations in the power stroke. The present study was concerned with assessing the possibilities for improvement through spark-electrode design. The study indicates that significant improvement would result from the use of electrodes designed to project ions (including free radicals) into the combustion chamber ahead of the flame front, since the transition from spark kernel to flame front tends to be relatively slow and variable under lean burn conditions. The results of the study are promising, and direct-funding support is being sought for detailed experimental verification.

Reference:

1. U.S. Congress Office of Technology Assessment, "Automated Guideway Transit — An Assessment of PRT and Other New Systems" (including supporting Panel Reports), June 1975.

BOX LAUNCHER DEVELOPMENT

The APL Experimental Development Model (EDM) Box Launcher has been tested successfully. Provisions for obtaining range time for the test were made with the assistance of the Standard Missile Project Office at APL and with the support of the SM-2 Navy Program Office.

APL has been engaged in the development of a universally adaptable box launcher for the Standard Missile family and future missiles similar in performance and configuration. Details were reported previously. A prototype of the box launcher was tested in 1969 and was approved by the Navy in 1970 for installation on 1052 class destroyers under the Interim Surface-to-Surface Missile Capability (ISSMC) Program. Following the ISSMC Program, APL continued development work on the box launcher to improve components, structures, and reduce cost. As a result, a second-generation Engineering Development Model (EDM) launcher cell was completed in June 1974 and a Blast Test missile was fired from it on 29 September 1975 at the White Sands Missile Range (WSMR).

It was planned initially to conduct a test firing from the EDM launcher during the spring of 1975 using a Blast Test Vehicle (BTV) airframe from parts at APL and equipped with a rocket motor constructed by APL and loaded with propellant by the Aerojet Solid Propulsion Company, Sacramento, California. However, the cost of loading one rocket motor was excessive and arrangements were made to purchase from Aerojet, at a reduced cost, a complete loaded motor assembly made from parts that would be fabricated during a production run for the Navy during 1975. The motor became available in early September and was shipped to WSMR for assembly into the BTV airframe in preparation for a test firing from the EDM launcher.

The test firing from the EDM was made on 29 September with the objectives of demonstrating functional operability, evaluating new and improved operating mechanisms, investigating shock and vibration effects on the elastically suspended launch rail system, and testing a new design of frangible forward and aft launcher closures. The test was completely successful. Extensive photographic data were obtained of the missile launch and disruption of the test closures. Shock and vibration data were also obtained from accelerometers mounted in the launch rail. A preliminary visual examination of the EDM launcher after the test disclosed no damage to operating components of the launcher.

Films of the tests were sent from WSMR to APL for analysis. The EDM was returned for disassembly and detailed study of blast effects on components and mechanisms. Following the test-data analysis a report will be prepared and recommendations will be made for future action on a box launcher design to meet full tactical requirements for shipboard installation. It is anticipated that the data reduction and report can be completed during the second quarter of FY 76. Direct Navy funding will be requested for the development and test work required to achieve a finalized design for tactical installation.

Principal Investigators: S. Kongelbeck and W. F. Williams. Mr. Kongelbeck is APL's Chief Engineering Consultant and Mr. Williams is Branch Supervisor of the Mechanical Engineering Branch of the Engineering Facilities Division.

THE JOHNS HOPKINS UNIVERSITY
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ATMOSPHERIC ELECTROSTATIC FIELD MEASUREMENTS

Stability of the electrostatic field of the earth is important to the DoD in connection with stabilization of remotely piloted aircraft. An investigation was devoted to the acquisition of electrostatic field gradient data during the flight of the Project Da Vinci manned balloon laboratory. The first flight test of an APL experiment package demonstrated overall success in design performance, but data interpretation was hindered by non-design deployment of other experiments aboard the balloon.

The balloon-borne manned laboratory established for the investigation of phenomena within a moving parcel of air in the lower atmosphere is known as Project Da Vinci. The laboratory has been sponsored by ERDA, the National Geographic Society, and the Army Atmospheric Sciences Laboratory. Some eighteen other laboratories, both U.S. Government connected and private, are participating in Da Vinci. The first flight of the Da Vinci balloon took place on 29 October 1974 from a launch site near Las Cruces, NM. The second flight of a modified and expanded program is expected to leave from a location in Oklahoma early in 1976.

Very little usable and reliable information on atmospheric horizontal potential gradients is presently available, so one purpose of the APL experiment was to ascertain the circumstances that cause horizontal gradients to reach a sufficient magnitude to interfere with the navigation of electrostatically stabilized RPV's (Refs. 1 and 2).

A dual-channel electrostatic field meter, designed and built at the Applied Physics Laboratory to measure vertical and horizontal components of the electric potential gradient in the atmosphere, was delivered to the Da Vinci assembly location at Kirtland AFB, Albuquerque, NM and installed on the gondola.

The balloon was launched at about 9:00 p.m. on 29 October with the APL experiment package deployed shortly after launch approximately 100 ft below the gondola on a Dacron line. The package functioned normally and usable data were generated. However, at about 1:40 a.m. of 30 October another larger instrument package (not a part of the APL experiment) was lowered on a line to the vicinity of the APL meter, causing an unacceptably large artificial horizontal disturbance of the electric field. Flight plans called for lowering this second package well below the APL instrument, but this was not possible because of other problems. So the situation continued for the remainder of the flight, which was terminated earlier than planned because of weather at about 8:00 a.m. 30 October near Wagon Mound, NM.

During the flight the APL package was rotated slowly about the vertical axis to provide sensing of horizontal components of the electric field in all directions and to give adequate ventilation to the radioactive sensor probes. A two-axis magnetometer on the package gave continuous information about the orientation of the probe antenna. Analog signals from the horizontal and vertical gradient voltmeters and the magnetometer were converted to FM multiplex and relayed to a recording station in a truck that attempted to follow the path of the flight along the ground.

Early in 1975 APL received the data tapes from the flight; results of initial analysis were issued in March 1975 (Ref. 3). Results of the analysis show a reasonable trace of vertical potential gradient as the flight progressed. Insofar as data could be analyzed, there appeared to be no horizontal gradients that would be large enough to cause notable disturbance of an electrostatically stabilized vehicle.

In March 1975, meetings were held at ERDA to discuss Da Vinci I results and to begin planning for Da Vinci II. The main purpose of the remaining flights will be the chemistry of sulfate pollution in the atmosphere in connection with combustion of fossil fuels. Continued participation by APL in the Da Vinci project could lead to development of air pollution monitoring and detection equipment based upon the principle of sensing atmospheric electric phenomena with lightweight and relatively inexpensive devices similar to those used in the electrostatic stabilization of Mini-RPV's, but future participation will be contingent upon receipt of direct funding.

Principal Investigator: M. L. Hill. Mr. Hill is Supervisor of the Aerophysics and Flight Research Group of the Aeronautics Division.

References:

1. M. L. Hill and T. R. Whyte, "Investigations Related to the Use of Atmospheric Electric Fields for Aircraft and RPV Stabilization," APL/JHU TG 1280, November 1975.

2. M. L. Hill, "Introducting the Electrostatic Autopilot," Astronautics and Aeronautics, Vol. 10, No. 11, November 1972, pp. 22-31.

3. T. R. Whyte, "Preliminary Analysis: First Da Vinci Flight," APL/JHU BAF-75-02, March 1975.

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AIR TRAFFIC CONTROL RADAR SURVEILLANCE

System concepts have been developed for conducting terminal airspace surveillance on a cost effective basis using radar in support of air traffic control during the 1980's.

Air traffic control is presently conducted in high-traffic-density terminal-control areas using surveillance systems that use both search radar and aircraft beacon transponder sensor subsystems. The signal returns from these subsystems are processed and correlated to establish and display the position histories of the aircraft, thus permitting the air traffic controllers to vector the pilots. A concept is under development for airspace surveillance in the 1980's that will use a next generation beacon transponder technique, Discrete Address Beacon System (DABS), as the primary sensor. This approach should offer a viable solution to air traffic control in high-density airport areas; however, it is judged that it will not satisfy all the air-traffic-control surveillance requirements. First, in high-density areas with DABS, a backup surveillance capability that does not depend on aircraft-installed support equipment will be required. Second, many terminal areas that will not require installation of this rather expensive next generation system will require a surveillance capability. Therefore, the Systems Research and Development Service of the Federal Aviation Administration undertook a study to guide future development of terminal radar-based surveillance systems.

The FAA requested the Mitre Corporation, Massachusetts Institute of Technology Lincoln Laboratory, and The Johns Hopkins University Applied Physics Laboratory to participate in this study by supporting their Radar Study Committee. The three organizations were chosen because of their background in applicable military and related FAA tasks. Because of the importance of the task and the unavailability of direct funding, the work at APL was supported by its IR&D funds.

The Radar Study Committee established two subcommittees, one to address surveillance for airports that would be equipped with DABS and the other to address airports that will not qualify for DABS because of lower traffic densities. The former system was identified as the DABS Backup Radar, while the latter was called the Short-Range Terminal Radar (SRTR). The SRTR subcommittee was chaired by Mr. D. B. Staake of APL, and most of the Laboratory effort was concentrated on this subtask. The DABS Backup Radar subcommittee was chaired by Mr. E. Muehe of Lincoln Laboratory.

The work of the two subcommittees resulted in the conceptual definition of two radar-based surveillance systems to satisfy

the stated requirements. The discussion to follow highlights the salient aspects of the SRTR portion of the study.

The primary operational requirements for a short-range terminal radar were identified as listed on the bottom of Table 1. Attention then focused on the definition of radar system parameters that would satisfy these requirements and be consistent with other influencing factors such as cost and ease of operating frequency allocation. The investigation resulted in three candidate systems, which are identified as a function of operating frequency across the top of Table 1. Each of the candidates has, in common, pulse width, pulse repetition frequency, and antenna beamwidths.

Analysis indicated that the ground clutter requirement for each candidate system was equivalent and that circular polarization to obtain required weather clutter performance was not required (i.e., linear polarization was sufficient). As operating frequency increases, RF power increases, antenna size decreases, and rain clutter improvement requirements become more stringent.

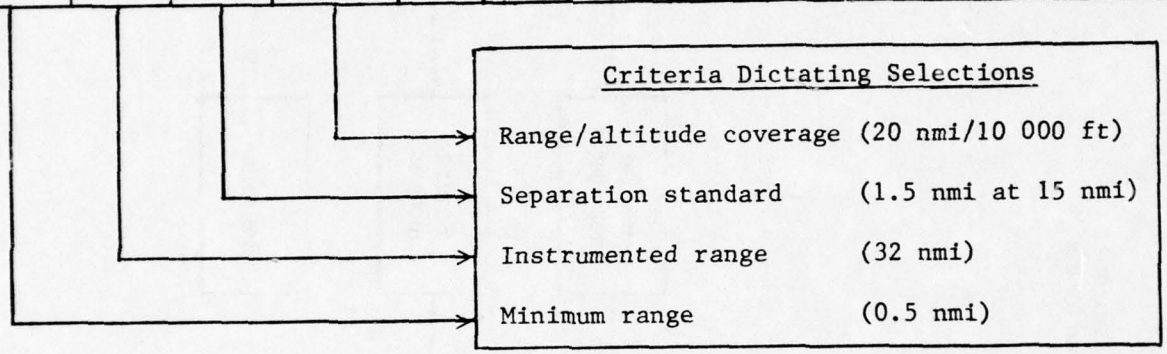
Figure 1 presents a functional block diagram of the resulting configuration for the three candidate systems. The dashed lines indicate configuration changes that are possible should the L-band candidate be implemented using a common antenna system with the existing L-band beacon surveillance subsystem.

Several new design approaches were used in the definition of the three candidate systems. First, the entire system, with the exception of the display in the control tower, is to be packaged using modular techniques in a self-contained unit. Such packaging will reduce maintenance and installation costs significantly. Second, a new two-channel video processor developed by Lincoln Laboratory, called the Moving Target Detector, would be used. This video processor has a significantly wider dynamic range than processors presently used,which will enable better performance to be achieved in the presence of clutter and possibly the display of more meaningful weather data. Last, the control tower display system is to be of the interactive graphics type, which will permit, among other advantages, a cheaper and easier installation of remote displays in the control tower, an easier display of weather information, and the presentation of aircraft tracks using scan history techniques.

The definition of these three candidate SRTR systems indicated that any of the three could be implemented with relatively low risk and cost. In addition, available technology should ensure that such systems would be highly reliable, thus requiring

Table 1
Radar System Candidates

*Frequency Band	Pulse Width (μs)	PRF (kHz)	Antenna Beamwidth		Power		Clutter Improvement Required		Antenna		
			Az. (deg)	El. (deg)	Peak (kW)	Avg. (W)	Rain (dB)	Gnd. (dB)	Width (ft)	Height (ft)	Polarization
L	2	2	3.4	0.5 to 20 CSC^2	8	32	7	38	15	14	Linear
S	2	2	3.4	0.5 to 20 CSC^2	59	236	21	38	7	6.4	Linear
S'	2	2	3.4	0.5 to 20 CSC^2	98	391	25	38	5.5	5	Linear



*L-band: 1.25 to 1.35 GHz
S-band: 2.7 to 2.9 GHz
S'-band: 3.5 to 3.7 GHz

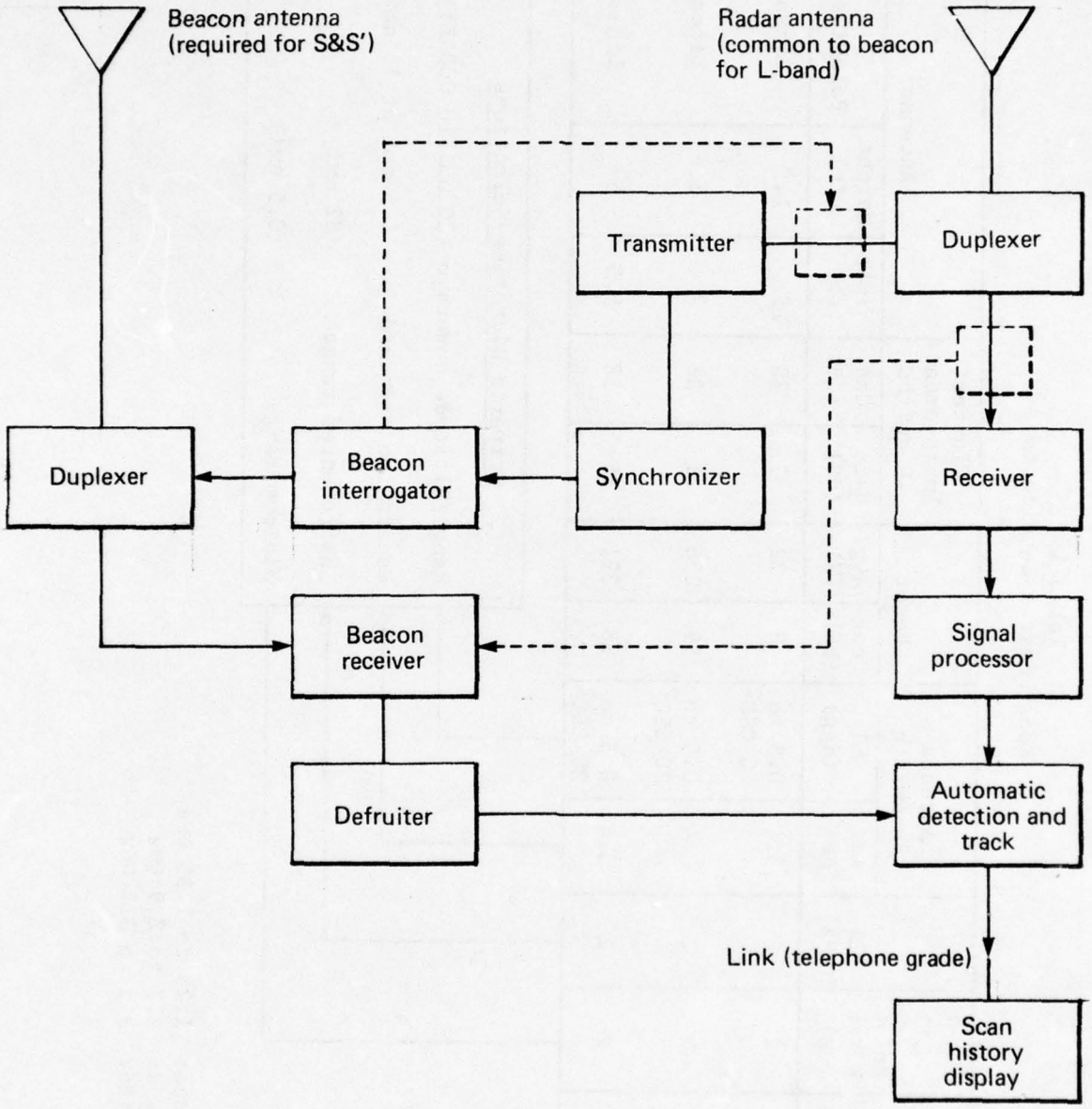


Fig. 1 Candidate Radar Systems, Block Diagram

low maintenance. These two highly desirable logistic support characteristics should be the result primarily of the modest RF power required, small antenna size, and solid-state modular construction. And finally, the life cycle costs for the three candidates should be roughly equivalent.

Consideration of operating frequency allocations, possible radio frequency interference problems, and proper use of the frequency spectrum indicates that the S' band candidate should be given preference.

The work on this project has been documented in draft form (Ref. 1), and a final report will be issued.

Principal Investigator: D. B. Staake. Mr. Staake is Branch Supervisor of the Operational Systems Development Branch of the Fleet Systems Department.

Reference:

1. "Short Range Terminal Radar," FAA-RD-75-7, 1 (Draft), January 1975.

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RADAR DETECTION OF TURBULENCE ASSOCIATED WITH THUNDERSTORMS

Severe thunderstorms and other weather phenomena represent a major problem in aviation safety, chiefly because of the adverse effects of associated turbulence. A study has been completed (Refs. 1 and 2) that reviews and evaluates research that has been done, and defines additional research that is needed to establish the use of radar for reliable detection of turbulence.

Turbulence is frequently present in the atmosphere and is usually associated with thunderstorms, but there is no satisfactory method at present of determining the location of these turbulent patches so that pilots could be warned of their presence. The only tactic available to air traffic controllers for complete safety is to avoid storm areas. However, in many instances, and in the vicinity of large airports in particular, it is not always possible for air traffic controllers to route airplanes around weather patterns. In 1974 the Federal Aviation Administration (FAA) expressed to the Applied Physics Laboratory an interest in developing techniques to detect and adequately display regions of turbulence within weather patterns. Because of the importance of this problem, and because APL has expertise in radar meteorology as well as in the application of adaptive techniques to radar data, a study was begun to apply this expertise to the solution of the turbulence detection problem.

Although turbulence associated with weather has been studied, it still is not completely understood. Methods of detecting it are still in the research stage. However, it has been clearly demonstrated that radar can detect clear-air turbulence where fluctuations in the refractive index, on the scale of one-half the radar wavelength, act as tracers of the air motions. Since radar is also effective in detecting hydrometeors associated with thunderstorms and clouds, it should also be capable of measuring such turbulence to the extent that the hydrometeors trace the air motion within the storm.

The problem has been that the reliability of radar echo parameters to indicate the presence of turbulence has not been determined. Atmospheric turbulence is the random fluctuation of velocities, and must be described statistically. The phenomenon spans several scales of turbulence; those scales that affect the aircraft depend on the characteristics of the aircraft (size, design, etc.). Hence any parameter that indicates turbulence must be of a statistical nature.

Incoherent Radar as a Turbulence Detector

Incoherent radar is the type most commonly available for detecting air turbulence. Its use was explored previously but results were disappointing. In principle, the variance of the spectrum of radar amplitude fluctuations is related to the rms fluctuations of velocity. The problem with incoherent radar is that its response is determined primarily by fluctuations of velocity components only on a scale given by one-half the radar wavelength. It has yet to be shown experimentally whether the measurement of any given scale will define adequately turbulence for other scales such as those of special concern for aircraft safety. However there is theoretical evidence that the spectrum of velocity fluctuations should follow a power law. Thus, if the theory is valid, then the entire spectrum of velocity fluctuations could be inferred from a measurement of velocity fluctuations on the scale of one-half of the radar wavelength. For this reason incoherent radar cannot be ruled out and experiments should be performed to determine its usefulness.

Doppler Radar as a Turbulence Detector

Doppler radar systems seem to be the most promising means for detecting turbulence because velocity fluctuations can be sensed over a wide range of turbulence scales. With single doppler systems, it is possible to measure the radial velocity of air motions (using the hydrometeors as tracers); with dual doppler systems, the two-dimensional vector velocity can be measured. As with incoherent radar, some experiments have been performed, but no definite turbulence parameter has been isolated. There are several potential parameters including, e.g., variance of the doppler spectrum, and the velocity gradient between two regions of space. None has been tested thoroughly to assess usefulness alone or in conjunction with other parameters.

Data Processing

The feasibility of optimal data processing is necessarily of concern when radar-derived parameters of a statistical nature must be displayed on a real time basis. Although the best method of processing turbulence data cannot be determined until those quantities to be processed are decided upon, it is found that mini-computers and advanced radar data handling techniques allow almost any parameter to be processed and disseminated in a manner easily understood by air traffic controllers or others needing the information. For example, until recently it was extremely difficult to determine accurately radial velocity in real time for large areas of the atmosphere. The reason is that, in the

past, radial velocities were obtained by spectrum analyzing the radar signal and computing the mean and variance of that spectrum, a process that entails storing large quantities of data and executing lengthy computations. In recent years this problem has been eliminated by using a correlation technique (pulse-pair processing) which allows fast, real time acquisition of radial velocity values.

Finally, an experimental program was defined (Ref. 2) to determine those radar derivable parameters that best indicate turbulence. The experiment could be performed at Wallops Island, Virginia (where APL has three high-power radars) using the Spandar radar to measure intensity and velocity in a three-dimensional storm pattern and an aircraft equipped with sensors to measure velocity fluctuations to confirm the validity of the radar data. These data would be recorded and analyzed to determine the turbulence parameters and to investigate adaptive techniques that could be used to develop a turbulence detection system.

In summary, the potential for radar in general, and doppler radar in particular, as a turbulence detector is good. The parameters that could be derived from radar data and used to indicate turbulence in a reliable manner should be determined by experiments as described in Ref. 2.

Principal Investigator: Ella B. Dobson. Mrs. Dobson is a senior mathematician in the Radar Atmospheric Physics Group of the Fleet Systems Department.

References:

1. "A Review and Study of Radar as a Turbulence Detector," APL/JHU F1E74U-058, 16 December 1974.

2. "Proposed Turbulence Experiment," APL/JHU F1E75U-002, 17 January 1975.

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VESSEL TRAFFIC SYSTEM

Improved vessel traffic monitoring and control is an important goal in both DoD and civilian areas. APL was a major participant in the development of the U.S. Coast Guard's San Francisco Experiment Vessel Traffic System, an all-weather radar/communications/computer/display complex used to advise mariners of traffic conditions within the area's deep draft waterway system. The project reported here builds on that experience to define advanced technical concepts for future Vessel Control Systems.

A unique aspect of the San Francisco Experimental Vessel Traffic System (VTS) was its extensive use of real time data processing technology. That installation (Refs. 1 and 2) demonstrated automatic detection and tracking of vessels within radar coverage areas, even in the presence of sea clutter (Ref. 3). Information on the movement of vessels was extracted from the radar signals, presented to operators on computer animated displays, and the traffic was analyzed both automatically and at the request of the operator (Ref. 4).

The present study was initiated to explore advanced concepts for future VTS systems (Ref. 5), and in particular, to define elements of a system suitable for deployment in the Port of Baltimore and its Chesapeake Bay approaches. Major objectives included use of economical commercial radars and computers, coupled with a reduction in operational manning requirements.

Vessel traffic systems are intended to minimize collisions, rammings, and groundings through computer-aided visual and radar surveillance, display, risk recognition, and management of vessel traffic. A comprehensive VTS design begins with an objective and methodical appraisal of the risk potential of the area in which the system would be used. Established patterns of movement define a track network. A quantitative risk associated with movements along each segment of each track is computed, and analysis defines regions that offer the greatest potential for mishaps, ranked in accordance with risk. This procedure leads to recognition of safe routings and speeds, and makes possible automated evaluation of risks associated with off-course errors.

The present study defined a modular system consisting of a traffic subsystem located at a central VTS management facility, a number of surveillance subsystems deployed at key sites in the bay area, plus data entry and communications capabilities. Significant departures from the approach employed in San Francisco were recommended, including the following:

1. Active Traffic Management in which departure, speed, and routing is adjusted to limit congestion in critical regions;

2. Telephone Data Links to remote radar sites, rather than microwave communications;

3. Enhanced Automatic Tracking capabilities through use of amplitude data, an integrated track file, and radar-site preprocessing; and

4. Reduced Manning Requirements via active participation of key maritime community elements.

Study outputs included lists of candidate surveillance sites, vessel movement reporting points, operator services, and computer-initiated alerts. A variety of other functional capabilities that should be considered for inclusion were also enumerated.

Documentation of the effort was forwarded to Coast Guard R&D and Engineering personnel. Additional copies defining Chesapeake Bay vessel traffic system requirements were subsequently requested for distribution to 5th Coast Guard District personnel.

Principal Investigator: A. J. Cote, Jr. Mr, Cote is a senior engineer in the Operational Systems Development Branch of the Fleet Systems Department.

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MICROPROCESSOR APPLICATIONS

A general goal of the microprocessor project is to develop an in-house capability in microprocessor applications to Laboratory projects. Two commercial microprocessors have been acquired and integrated into several systems to study their capabilities and limitations. Because of the exceptional versatility of these devices, continuing studies are expected to provide the Laboratory with a valuable capability in the new technology.

Very small-scale computing devices appeared in the marketplace about 1972, but were of limited capability. By 1974, several microprocessors were developed that seemed to offer sufficient computational power for tackling nontrivial applications. To exploit this new potential, the microprocessor project was established to develop a familiarity with these devices and a capability for applying them to operational systems.

IC-8080

One of the devices initially investigated was an 8-bit processor-on-a-chip manufactured by the Intel Corporation, the 8080. This device is already available from at least two vendors and is in the Navy Standardized Electronic Module (SEM) program in Mil. Spec. versions. At least four other projects within APL benefited directly from this investigation; one of them has adopted the 8080.

An important milestone was successful integration of the microprocessor in both hardware and software aspects, with an available high-speed paper-tape reader. With the support software (a text editor and an assembler) available, software could be developed with low-level languages. Next, a plasma display device was connected to the microprocessor and elementary supporting software was written. Thus two radically different devices were readily interfaced to the processor. This feature alone makes the device of interest to a large segment of the logic design and system design communities.

Many studies of software cost and reliability have demonstrated the advantages of using a higher-level language for programming. The IC-8080 has such a language, and its capability was successfully demonstrated. Two test programs of moderate complexity were written in the higher-level language, translated into machine's language by the IBM 360/91, and executed on the microprocessor. (The use of a large host computer is required because of the limited capabilities of the microprocessor itself.) The

higher-level language itself has been found to be quite useful and is now the more popular language.

Two further milestones have been reached, both dealing with interfacing the microprocessor with a computer. The first microprocessor/computer link was established with the IBM 360/91. The object of this connection was to facilitate transmission of microprocessor programs written in the higher-level language and translated by the IBM 360/91. Another microprocessor/computer interface was made with a minicomputer, the Alpha LSI. This latter link is operational at the hardware level, but software is incomplete. The purpose is to demonstrate the effectiveness of a multiprocessor/computer configuration. The ultimate system architecture would have several microprocessors and one minicomputer. Each microprocessor would perform a local control function such as closing a servo loop or operating a printer while the minicomputer would control the microprocessors in some system-wide optimum manner.

IMP-16P/308

Another microprocessor investigation focused on the National IMP-16P/308 Prototyping Microprocessor System that was delivered on 20 December 1974. The IMP-16P/308 is a complete microcomputer prototyping system that allows program and hardware development for the IMP-16C (16 bit) microprocessor card. Investigation in software development resulted in the procurement and installation of the IMP-16 Conversational Assembler and the IMP-16 Off-Line Cross-Assembler programs. The first operates on the IMP-16P microcomputer and is used for on-line program assembly and editing. The second is a cross-assembler residing on the IBM-360/91 and is used for off-line program assembly. Both assemblers were successfully demonstrated and used.

The main objective of this project was to make a microprocessor system available for familiarization and system development work. After checkout and interface with a teletype, the IMP-16P/308 system was almost 100% available for use in direct funded programs. It is noteworthy that an initial limitation of the IMP-16P/308 system was its slow input speed through the teletype. As part of the IMP-16P/308 interface investigation, a magnetic tape input interface was implemented, thus improving the system input rate by a factor of 10 or so.

Since its installation, the IMP-16P/308 has been used in a number of diverse applications. With assistance from APL staff members, Dr. Alan Zuckerman of Johns Hopkins Hospital performed

the masking (programming) of the PROM memory to be used in an IMP-16C microprocessor, a component part of a new pulmonary function screening system. The IMP-16P/308 system was also used extensively in the development of the PROM's for the IMP-16C used in the Transim, a low-cost satellite navigation system; and the APL Mechanical Fabrication Division used the system extensively in the preparation of pumched-paper tapes for a newly acquired digitally-controlled milling machine.

Summary

The general goal of the microprocessor project is being achieved. Capability for using these very small computing devices has been demonstrated via several projects encompassing both software and hardware facets. It is expected that the equipment now on hand will serve a steadily increasing number of users and that additional devices will be acquired in order to stay abreast of the state of the art.

Principal Investigators: M. J. Gralia and S. Tsakos. Dr. Gralia and Mr. Tsakos are senior engineers of the Operational Systems Development Branch of the Fleet Systems Department.

NAVY SATELLITE COMMUNICATIONS

The general objective of this project was to examine satellite communications technologies and system concepts that could provide the Navy with an enhanced satellite communication capability to meet the present and projected requirements, while continuing utilization of the planned ultra-high frequency (UHF) and super-high frequency (SHF) terminal equipment. Alternative satellite constellations were examined and a conceptual design of the satellites has been defined for two candidate systems.

The Space Development Department, with the assistance of other portions of the Laboratory, has performed studies of Navy communications by satellite. The studies consisted of two separately defined and separately supported complementary parts; the analytical aspects of the work were performed with IR&D funds, whereas the engineering studies were direct funded by the Navy. Conclusions from these studies are listed below; details have been published elsewhere.

Of the satellite systems examined, one is a conventional 1 × 4 ring of synchronous equatorial satellites, and the other is a 2 × 4 constellation containing two orthogonal polar rings, each with four satellites in circular orbit at an altitude of 4503 nmi (and with orbital periods a little less than five hours). The two systems would be capable of providing operational service starting in the early 1980's and represent second-generation replacement candidates for the FLTSAT I system. The satellites in both constellations incorporate design features to enhance jamming resistance, increase traffic capacity, improve connectivity, and permit central control of the system.

Candidate constellations were compared, using FLTSAT I as the baseline for capabilities and costs, to determine the optimum system for the Navy. The primary conclusions are as follows:

1. In the comparison of the synchronous, subsynchronous, and FLTSAT I constellations, it is evident that the synchronous and subsynchronous systems offer better communication capacities than FLTSAT I, and of greater importance, the SHF communication services (provided by steerable spot beams) of the second-generation systems are highly resistant to enemy uplink and downlink jamming. Crossbanding of the UHF and SHF communications is an inherent capability of both second-generation systems.

2. A subsynchronous, polar-inclination satellite constellation offers several advantages over a synchronous constellation in global coverage, jamming resistance, and communication effectiveness including any periods of satellite signal outage. The failure of an equatorial satellite at synchronous altitude results in loss of service over nearly one-fourth of the covered surface of the earth. This outage may last for a period of a week or more until an in-orbit spare can be brought on station. A superior adaptation to satellite failure is provided naturally by the constellation of subsynchronous satellites. No fixed geographic region completely loses service during the outage period at a single orbiting station. Furthermore, the size of the everchanging geographic region that is not covered because of the outage is much smaller than in the case of the synchronous equatorial constellation. At latitudes above 40° no outage occurs as the result of one satellite failure.

3. A constellation of second-generation synchronous satellites designed to the cost of FLTSAT I (176 million dollars) would provide only one-half the UHF capacity and one-quarter the SHF capability assumed to be required to serve the user communication terminal equipment planned for Fleet deployment in the 1980's. The constellation of subsynchronous satellites, designed to the same cost, has the full UHF and SHF capacities to meet these assumed needs for all the planned users in the 1980's. It is estimated that a subsynchronous constellation, providing the same service as a synchronous constellation, would cost one-half as much.

4. The post-launch operations and routine tracking of a subsynchronous satellite constellation can probably be accomplished by the existing CONUS facilities of the Navy Astronautics Group without interfering with the Transit system. Optional stations may also be established at sea or overseas. Although the tracking of the synchronous satellites can possibly be performed from CONUS using the satellite-to-satellite link, post-launch operations in deploying replacement synchronous satellites will probably require overseas stations for tracking, telemetry, and control.

5. Neither the synchronous nor the subsynchronous system require CONUS satellite communication ground stations. However, each is compatible with communication operations with such stations.

6. Division of the satellite UHF downlink carriers among several antennas and reduction in the number (compared to FLTSAT I) and selection of downlink frequencies will eliminate intermodulation self-jamming of the UHF uplink receivers. Multiplexing of the downlink carriers can be used to provide greater Navy traffic capacity from the reduced number of carriers.

7. Economy in satellite manufacture can be obtained from the use of solar power arrays using reflectors that increase the intensity of illumination on the silicon solar cells and reduce the number of cells required. Also, the use of solar concentration permits the use of thick cover glasses over the cells to provide radiation resistance.

8. Three-axis attitude control of a subsynchronous satellite to provide the required orientation of the communication antennas and the satellite-to-satellite data link antennas can be accomplished by techniques proved in the Transit, Small Astronomy Satellite (SAS), and Geodynamic Experimental Ocean Satellite (GEOS) Programs. These techniques require no expenditure of propellant and therefore do not limit service life.

9. No new technology is required in the satellite designs considered. Hardening and reliability measures established in the previous and current Navy and NASA satellites appear to be directly applicable. A service lifetime comparable to commercial communication satellites (i.e., 8 to 10 years) should be realized.

Principal Investigator: T. Wyatt. Mr. Wyatt is a senior engineer in the Space Department Office.

SPACE RESEARCH AND TECHNOLOGY

The Laboratory has long been active in space-related science and technology through directly funded DoD and NASA programs. Characteristically, however, such programs tend to emphasize state-of-the-art knowledge. Accordingly, a small but continuing, indirectly funded effort has been devoted to enhancing vitality and advancing state-of-the-art knowledge in these areas.

Over the years, indirectly funded exploratory research and development at APL has led to many significant advances in space-related science and technology. Technologically, the most significant advance was the concept that led to the present Navy Satellite Navigation System. More recently, instrumentation development included the first satellite-borne solid-state detector and also the longest lived solid-state detector system, still functioning after more than 12 years in orbit. Recent scientific achievements include the discovery of field aligned currents in the ionosphere and the development of increasing understanding of their effects on radio communications.

During the current period, work has been performed and significant new results have been achieved in areas of (a) spacecraft data analysis, and (b) satellite instrumentation. These include the discovery of a new region of field-aligned currents that appear to be involved in coupling between the interplanetary medium and the magnetosphere of the earth, and also the characterization of the response of various thin-film scintillators to low-energy particles. Additionally, (c), a new project in radio-astronomy has been initiated in collaboration with COCOA-Cross radio-telescope scientists.

Analyses of Spacecraft Data

Disturbances of the earth's magnetosphere and ionosphere are important for several reasons, including their disruption of DoD and civilian radio communications. Many spacecraft provide unique data that can contribute toward understanding and predicting these phenomena. Using IR&D funds, the Laboratory has for many years supported a low level of effort directed toward these ends; many significant results of this work have received international recognition.

During the present period, emphasis has been placed primarily in two areas, analysis of TRIAD magnetometer data and continued analysis of Interplanetary Monitoring Platform (IMP) energetic particle data.

Field-Aligned Currents. The Navy/APL TRIAD satellite provides the only extensive vector magnetic field data for the inner ionosphere. These data have been undergoing analysis at APL for several years. During the present period, the study has been performed primarily by Dr. Iijima, a Postdoctoral Associate on leave from the University of Tokyo. The results reveal that the magnetosphere-ionosphere current system, which contains field-aligned currents, consists of two distinct parts. The first part, located at the high-latitude boundary of the auroral region, is permanent. The second part, located at the equatorward boundary of the auroral region, is variable, and is an important element of the auroral electrojets. The total magnitude of these currents varies between 10^6 and 10^7 A depending upon geomagnetic activity. Dr. Iijima has recently discovered a region of field-aligned currents that is located within the region associated with the dayside magnetospheric cusps. The relationship of the intensity of these currents with interplanetary magnetic field values suggests that they may play an important role in the coupling between the interplanetary medium and the magnetosphere. Dr. Iijima has also correlated field-aligned current distributions determined from 1400 TRIAD passes with the global distribution of ionospheric currents in the polar cap. The results of this study indicate that the field-aligned currents, located at the polar boundary of the auroral region, are a permanent feature of the three-dimensional current system coupling the magnetosphere and ionosphere. They are dependent upon ionospheric conductivity in addition to polar geomagnetic activity. The source of these field-aligned currents appears to be associated with the dayside magnetospheric boundary where the geomagnetic field lines have continuous and free interaction with the solar wind and interplanetary magnetic field.

During his visit at APL, Dr. Iijima has co-authored two manuscripts that have been accepted for publication and is presently preparing two more. He has participated in seven papers presented at the spring and fall American Geophysical Union meetings, the Conference on Quantitative Magnetospheric Models in La Jolla, California in May 1975, and the XVI General Assembly of the International Union of Geodesy and Geophysics in Grenoble, France in August 1975.

Energetic Particle Analysis. During the present period, this phase of the data analysis effort has been carried out primarily by Dr. E. T. Sarris, a Postdoctoral Research Fellow at the Laboratory. He has been working primarily with energetic particle data from APL experiments on IMP (Interplanetary Monitoring Platform) satellites 6, 7, and 8. Simultaneous measurements of energetic protons ($E_p \geq 0.21$ MeV) by the APL instruments on board

satellites IMP-6, -7, and -8 show that (a) proton bursts are observed simultaneously (±30 min) inside the magnetosphere, in the magnetosheath, and upstream from the bow shock in association with the expansive phase of magnetic substorms. Therefore the magnetospheric bursts everywhere are part of one global phenomenon with a common origin. (b) Proton bursts are not observed inside the tail lobes at large distances ($|Z_{SM}| > 10\ R_e$) from the neutral sheet. (c) The highest proton intensities during proton bursts are observed in the vicinity of the neutral sheet.

On 16 October 1973, a magnetospheric burst was observed in the magnetotail simultaneously by the IMP-6 and -7 satellites while a magnetic substorm was in progress. The two spacecraft were only $\approx$ 1 R_e apart along the Y_{SM}-axis ($\Delta X_{SM} \simeq 1\ R_e$, $\Delta Y_{SM} \simeq \Delta Z_{SM} \simeq 0\ R_e$). Proton anisotropy measurements during this unique occurrence show earthward fluxes at both spacecraft at first, then earthward fluxes at the near earth spacecraft and tailward fluxes at the spacecraft further out, and finally tailward fluxes at both spacecraft. The sequence of anisotropy observations during this burst indicates the detection of the possible locus, size, and movement of the "source" of energetic particles in the magnetotail.

Results of this work have been published in two brief manuscripts and presented in six papers at scientific meetings. A comprehensive description has been submitted for publication and another is in preparation.

New Satellite Instrumentation

Support from IR&D funds allows a small continuing effort in research and development directed toward future spacecraft experiments, making it possible to remain at the forefront of experimental space research. Instruments developed here are well designed, reliable, and operate at or near the state-of-the-art. We have pioneered in the use of solid-state detectors, with both the first solid-state detector ever flown on a satellite, the APL INJUN I experiment, and the longest-lived 1963-38C, which contains detector systems that are still operational after more than 12 years. A complex MJS-77 experiment is the most recent product of our advances in the use of very thin detectors (2 μm), ultra-low-noise electronics, and hybrid circuitry. Recent efforts in the evaluation and development of new detector techniques have concentrated on time-of-flight measurements in particle detector telescopes, and on the development of suitable thin front elements for such telescopes. We have developed and explored thin-film ($\lesssim 25\ \mu g/cm^2$) scintillator technology for future use in flight applications, and have developed and successfully proposed for

the high background flux environment of the Electrodynamics Explorer Mission, a three-parameter particle telescope based on a first-element mosaic of very thin solid-state detectors and precise time-of-flight measurements.

At present a small ongoing development program, aimed at extending time-of-flight technology to even lower energies, is exploring the applicability of secondary emission foils as a front element in flight-qualified particle telescopes. Since direct funded projects are committed specifically to the production of flight hardware, the support for advanced development provided by IR&D funds is extremely important to continuing vitality.

Radio Astronomy — COCOA-Cross Collaboration

A two pronged collaborative effort was initiated during the current period with scientists operating the COCOA-Cross radio telescope. One part of the effort is a study of interplanetary scintillations, the other part deals with improved data acquisition.

Interplanetary Scintillations (IPS). An analytical study was begun in the hope that prediction techniques could be developed on arrival of geomagnetic and ionospheric disturbances. Gotwols and Roelof (of APL) working with Cronyn, Erskine, and Shawhan (University of Iowa) have analyzed 8 months of IPS observations taken in 1974 on the COCOA-Cross radio telescope. The IPS measurements were merged (Roelof et al., 1975) with Hα solar structure and interplanetary particle data to infer the three-dimensional configuration of the interplanetary medium. With the observation of over 100 IPS sources per day, the array can map interplanetary turbulence throughout the north ecliptic hemisphere and parts of the south ecliptic hemisphere. In an analysis of 20-30 June 1974 it was shown that a propagating interplanetary disturbance front could be seen approximately 6 hours before it engulfed the earth. IPS data, when combined with Hα and 0.3 to 0.5 MeV proton data from the APL experiment on IMP-7 (Explorer 47) in a simulated prediction of solar fluxes, revealed the three-dimensional configuration of the interplanetary medium and predicted a storm sudden commencement and delayed particle event 6 hours before it reached the earth.

A statistical study (Gotwols et al., 1975) of the variations in scintillation indices revealed a tendency for the scintillation index of a source at small solar elongation angles ($\leq 40°$) to be depressed, while simultaneously a source at the same longitude but at high latitude is enhanced. This is tentatively interpreted as a saturation effect, i.e., the source at small solar

elongation is in the strong scattering region where an increase in turbulence results in a decrease in scintillation. This saturation effect may account for the occasionally observed situation where sources separated by $\leq 10°$ show significant differences in their scintillation indices.

D. G. Mitchell (University of New Hampshire, Ph.D. dissertation, 1975) and Roelof have completed a detailed analysis of the analytical representation of the power spectrum of interplanetary radio scintillations (in the weak scattering approximation). The computational improvement is so considerable that extensive modeling of the response of the interplanetary medium in radio scintillations can be performed on a computer considerably smaller than the CDC 6600 previously required.

Data Acquisition for the COCOA-Cross Telescope. The COCOA-Cross radio telescope routinely monitors the interplanetary scintillation (IPS) of radio sources. However, data must be acquired in the presence of sharp noise spikes arising from terrestrial interference. Thus, there would be considerable advantage to using a minicomputer to recognize these noise spikes and replace them with data obtained by extrapolation between nearby interference-free data. Once this has been accomplished, the data rate can be compressed by a factor of 10 while still retaining all of its usefulness to the IPS study.

During the past year, a Nuclear Data 812 minicomputer was obtained on indefinite loan. It is planned to send this minicomputer to the Clark Lake Radio Observatory to serve as a "smart" data acquisition system in conjunction with the COCOA-Cross radio telescope. Several algorithms (digital filters, etc.) were developed for processing the data once the noise spikes have been "cleaned up". However, the exact criteria for identifying interference is still under study (because of the log-normal nature of IPS, the scintillations tend to be spiky, so great care must be taken in distinguishing between these legitimate spikes and interference spikes). Analog signal conditioning equipment was designed and built at APL and sent to the COCOA-Cross to allow analog tape recordings of the IPS signals to be made. These tape recordings allow the interference to be studied with the full gamut of instrumentation available in our laboratory. When this study is complete the interference rejection algorithm will be written, the remaining equipment interfaced, and the computer sent to Clark Lake to begin its observing chores. Beside allowing us to see between the occasional interference, this system will provide digital data with sufficient time resolution to allow power spectrum analysis, a major improvement over the analog chart recorder scheme now in use.

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Principal Investigators: S. Krimigis, T. A. Potemra, E. C. Roelof, B. C. Gotwols, T. Iijima, and E. T. Sarris. Dr. Krimigis is Group Supervisor; Drs. Potemra and Roelof and Mr. Gotwols are senior staff members; and Drs. Iijima and Sarris are postdoctoral appointees; all of the Space Physics and Instrumentation Group of the Space Development Department.

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ENVIRONMENTAL IMPACT EVALUATION

In recent years, this Laboratory has pioneered in the development of techniques for predicting and evaluating the environmental impacts of proposed electric power generating installations through studies carried out for and funded by the State of Maryland. The present IR&D project shows that such techniques can be extended and adapted to predict the impact of proposed on-shore oil production facilities. The project also assisted State of Maryland legislative committees in framing the coastal Facilities Review Act which became law in May 1975.

Predicting and evaluating the environmental (and social) impacts of large industrial/utility installations poses a great variety of unsolved problems. The methodology for coping with such problems is still in its infancy. In recent years, APL has acquired recognized competence in environmental impact evaluation through participation in the electric power plant siting program of the State of Maryland. Therefore, it is worthwhile to consider whether methodology developed for electric power plant evaluations can be usefully generalized and extended to apply to extensive petroleum-related installations of the kinds that have been projected for much of the East Coast. Problems posed by on-shore oil production facilities are particularly timely because of state legislation proposed for early 1975. Accordingly, an IR&D study project was initiated during the last weeks of the previous fiscal year and completed early in the present period.

This study consisted of comprehensive surveys of the environmental problems related to on-shore support facilities for off-shore drilling, transportation of crude oil, refinery and finishing plants; and in addition, reviewed the available technologies for the control of oil spills. The general approach to cost-benefit analysis was also outlined. It was concluded that much of the methodology that has been developed in the Power Plant Siting Program would also be applicable to impact prediction for oil support facilities. A report was issued in July (Ref. 1) which was well received, attracting considerable attention in this country and also abroad. In this connection, it is noteworthy that in part due to the acceptance given (Ref. 1), this Laboratory was asked by the FEA to carry out a Regional Pilot Study for the National Energy Siting and Facility Report. The Pilot Study was completed in the last month of this fiscal year, and the results are available in report form (Ref. 2).

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OCEAN THERMAL POWER PLANTS

An exploratory study of the use of solar energy through Ocean Thermal Energy Conversion (OTEC) shows that installations using state-of-the art technology could be operable within the next decade to produce huge quantities of energy-intensive products at costs that would be competitive with present methods which depend on diminishing fossil fuel resources.

As U.S. fossil fuel resources, especially natural gas and oil, decline it becomes increasingly important to develop solar energy systems. Such systems offer many environmental advantages in addition to "free fuel." A very attractive system would use the sun-warmed surface layer of tropical oceans and cold water from a 2500-ft depth as the heat source and sink to run a closed-Rankine-cycle system including a turbogenerator to develop electric power. Hydrogen could be generated by electrolysis of water, liquefied, and shipped to U.S. ports as a fuel. Even more attractive for the near term would be the use of the gaseous hydrogen at the floating plant with nitrogen from the air, to make ammonia. Available projections indicate that by 1985 the U.S. demand for ammonia will exceed the 1975 U.S. supply (presently made from our most scarce energy resource, natural gas) by at least 10 million tons. Our study indicates that this projected increase could be provided by 21 floating plants each generating 500-MW_e of power.

The APL concept for an OTEC/ammonia plant-ship is centered around an economical design of heat exchangers using large-diameter aluminum tubes. Ammonia is used as the working fluid to drive the turbine. The choice of using aluminum as the heat exchanger material and a plant-ship design, in which the heat exchangers are submerged in the ocean to provide approximately half of the necessary buoyancy for the plant-ship, lead to considerably lower costs than the "baseline" titanium-tubed heat exchangers housed within many-decked hulls proposed recently by industrial teams headed by TRW and Lockheed (Ref. 1).

A computer program has been developed for analysis of the proposed heat exchangers, which operate with two-phase flow of the ammonia inside multiple-pass (folded 20 or more times) tubes. Sea water flows from head ponds over these evaporators, then downward in a single pass between the tubes. It is then discharged below the ship where it sinks to a level where its density matches the local sea water density (a depth of about 200 ft for the warm sea water flowing through the evaporators and 1000 ft or more for the cold sea water that flows through the

condensers). Our tentative estimate for cost of producing ammonia at sea and delivering it to shore is approximately $70/short ton, compared to recent "plant gate" sales prices of $145-165/short ton for ammonia made from natural gas. Since the cost of natural gas and the demand for ammonia surely will rise, the OTEC/NH_3 plant should be competitive in the 1980's even if this tentative estimate were in error by a factor of more than 2. The estimate for liquid hydrogen, delivered to shore, is $5/million Btu and is less than half the recent sales prices. Manufacture of aluminum, magnesium, and other energy-intensive products is also being considered.

The Laboratory has attained significant stature in the OTEC field as a result of these exploratory OTEC studies (initiated during the previous reporting period). Eight papers (Refs. 1 through 8) have been published and three contracts have been obtained. In February 1975, APL was selected by ERDA to run their third OTEC Workshop; the proceedings (Ref. 1) were published in August. In April the U.S. Maritime Administration (MARAD) sponsored, at APL, a more thorough engineering and economic feasibility analysis to investigate the maritime construction, operation, and raw-material, product shipping aspects of plant ships based in tropical oceans (Ref. 9). In June ERDA requested a more detailed analysis of the heat exchangers and a proposal for conducting a follow-on experiment on the heat exchangers at the APL Propulsion Research Laboratory (Ref. 10). A small continuing exploratory study is planned to address certain special aspects not envisaged in present MARAD and ERDA sponsorship.

Principal Investigators: G. L. Dugger, W. H. Avery, H. L. Olsen, W. B. Shippen, and E. J. Francis. Dr. Dugger is Asst. Division Supervisor, Dr. Avery is Division Supervisor, Dr. Olsen is senior physicist, and Mr. Francis is executive assistant of the Division Office, and Mr. Shippen is Group Supervisor of the Propulsion Group; all of the Aeronautics Division.

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SOLAR CELL RESEARCH

Copper sulfide/cadmium sulfide (Cu_2S/CdS) solar cells are advantageous from the standpoint of ease and economy of fabrication. However, cells made by present techniques suffer from two serious faults, poor efficiency and degradation of performance with time. An exploratory investigation was made to determine whether sputter ion mass spectrometry of such cells would be valuable for understanding and hopefully alleviating their major faults.

Recent cost analyses have shown that, for the Cu_2S/CdS system to be "economical" when compared to other energy systems, the Cu_2S/CdS solar cell efficiency must be greater than 10%, whereas typical efficiencies are 5 to 6%. Theoretically there are no physical reasons for not achieving an efficiency of 10% in the Cu_2S/CdS system; in fact, several studies predict efficiencies of up to 18% (AMI). V_{oc} (open circuit voltage) appears to be the major cell parameter where an improvement could be achieved. V_{oc} for a typical cell is approximately 0.5 V; theoretically it can be as high as 1.2 V (i.e., difference in band gap between Cu_2S and CdS). It has been predicted that V_{oc} could be improved by reducing interface trapping states (dislocations) at the junction by proper doping. Reduction of trapping states would also improve the degradation problems if the assumed mechanisms are correct,

For terrestrial applications of Cu_2S/CdS solar cells, the strongest lifetime degradation factor is temperature followed by ambient gas and light exposure (i.e., spectrum, cycling rate, etc.). The degradation mechanisms may be attributed to one or more of the following parameters and/or processes: surface oxide and hydrate formation, bulk impurities in both Cu_2S and CdS, impurity diffusion in Cu_2S and CdS, and strain (or dislocations produced by lattice mismatch, etc.). These effects are usually lumped under two general categories: (1) surface, and (2) junction effects. Surface effects will be controlled by a proper protective coating once the mechanisms (species) are isolated. Hopefully, junction (bulk) effects will be eliminated or minimized by proper cell preparation and controlled doping.

Both the efficiency and the useful life of Cu_2S/CdS solar cells depend on the concentration profile of desired species and impurities through the thin (10 to 30 μm) layers of the cell. The sputter ion mass spectrometer (SIMS) is an instrument for obtaining microscale compositional profiles by using a beam of high energy ($\approx$ 10 keV) argon ions to sputter off the surface and a double focussing mass spectrometer to analyze the products. The mass-spectral intensities can be converted to concentrations by applying

sputter ion yield factors determined from the particular experimental conditions. Thus, the SIMS is found to be a valuable instrument for developing a detailed understanding of the performance of solar cells.

SIMS was used to analyze Cu_2S/CdS solar cell samples obtained from the University of Delaware (Ref. 1). The basic samples included: an as-evaporated CdS layer, a Cu_2S/CdS sample removed after barrier formation (i.e., topotaxial growth of Cu_2S layer by dipping the CdS into a copper chloride solution), and a Cu_2S/CdS sample subjected to a simulated gridding and lamination process. SIMS analysis resulted in a tractable number of species with observable differences in constituent profiles (e.g., Cu, Cd, and S) caused by processing. Typical profiles are shown in Fig. 1. Changes were attributed to the formation of the species $Cu_2SO_3 \cdot H_2O$ on the cell surface, CuS or CuO at the end of the Cu_2S barrier layer, and CdO at the original CdS surface before topotaxial growth.

Both the Cu_2S and CdS layers were found to contain impurities such as Fe, Mn, Li, Na, Ca, K, and Si; such impurities are potentially very important to the operation and stability of Cu_2S/CdS solar cells. Several of the above species, e.g., Na, K, and Fe, could act as dopants for the CdS and thus slow the diffusion of copper into the CdS, i.e., act as a diffusion barrier. Diffusion of copper into the CdS (and analogously Cd into the Cu_2S) is viewed as one of the major junction instability mechanisms in Cu_2S/CdS cells.

It was also observed that the concentration of $CuOH^+$ increased with time, possibly indicating the introduction of H_2O during prolonged exposure to the atmosphere. Profiles of $CuOH^+$ as a function of depth may be of interest in establishing the effect of the ambient on these cells. Oxygen is another species that should be investigated in great detail.

Principal Investigators: H. K. Charles, Jr., and F. G. Satkiewicz. Dr. Charles is a senior engineer of the Advanced Technology Project of the Engineering Facilities Division. Dr. Satkiewicz is a senior chemist in the Solid State Group of the Research Center.

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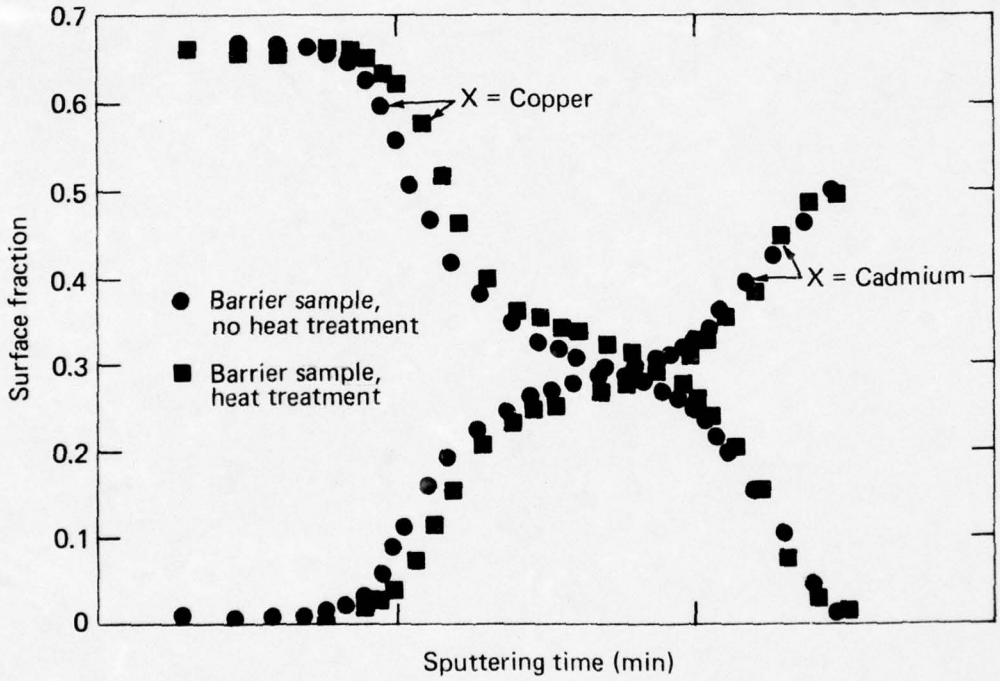

Fig. 1 Average Copper and Cadmium Profiles from SIMS Analysis of Cu_2S/CdS Solar Cell Samples 262C

INERTIAL ENERGY STORAGE

The Laboratory has developed a family of flywheel configurations based on the optimum use of high-performance anisotropic filament and composite materials. These flywheels appear to be capable of storing more energy per weight, volume, and unit cost than any other known type. Studies indicate widespread applications of these concepts for both DoD and civilian areas; e.g., in utility company peak-load compensating equipment, to have a significant effect on the national program of energy independence.

For several years, APL has supported studies under a low level of effort to explore the potentials of inertial energy storage. These studies show that advanced flywheel-type inertial-energy-storage techniques would be advantageous with respect to the amount of energy stored per weight, volume, and unit cost, and the Laboratory is a recognized authority in this area. The present IR&D program terminated in March 1975 when another source of funding became available.

The thin-rod and thin-ring Superflywheel configurations covered in previous reports have been analyzed to determine their applicability to various energy conservation programs, and especially to those programs connected directly with the utilities industry. Of particular interest is the implication that the use of these flywheels in lieu of future gas-turbine diurnal and load-following peak-load installations could eliminate the need for these gas turbines, along with their dependence upon an unstable fuel supply. The use of Superflywheel energy-storage systems instead of the turbines would not only substantially reduce the fuel requirement, but would reduce the cost of producing this peaking power by nearly an order of magnitude. The fuel-use cost of the gas turbine can be 10 to 20 times the fuel-use cost of the nuclear-base-load utility plants, which would provide the energy to be stored in an equivalent flywheel system. However, at the present time, the base-load plants are predominantly fossil fueled, and thus are only 5 or 10 times more fuel-effective than the gas-turbine peaking units.

The applications studies also showed that the very high power density, the instant-response, high-efficiency, scalability, and intrinsic reliability of the flywheel could permit additional economies to be realized that would not be possible with gas-turbine peaking plants. Properly exploited, these economies in associated equipment and improvement in efficiency of operation can amount to dollar values that total about 50% of the nominal installed cost of the flywheel peak-load compensating equipment.

The studies thus indicated that the flywheel peak-load compensating equipment, which was already cost-competitive with other proposed future peaking systems, is now felt to be improved in this category nearly 100%.

In view of the results of these studies, a program was established to obtain adequate government R&D funding for demonstrating the feasibility of these APL flywheel concepts. A number of government-related Superflywheel presentations were given in pursuit of this objective, and eventually an unsolicited R&D proposal was submitted to the National Science Foundation. (This proposed program was approved by NSF subsequent to the close of this reporting period.)

Principal Investigator: D. W. Rabenhorst. Mr. Rabenhorst is a senior engineer in the Space Development Department.

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SMALL-CAR STUDY

A brief exploration of the potential of increased use of small cars examines the effect on energy consumption and other secondary advantages and disadvantages. Three major questions were considered:

1. *How small is the smallest practicable car?*
2. *How would various Federal policies effect a transition to such small cars?*
3. *What transportation and economic effects would result?*

This study, initiated to response to an inquiry from a member of the U.S. Senate, differs essentially from studies elsewhere by considering the energy that may be conserved by encouraging a widespread transition to small cars in the range of 1000 to 2000 lb. The impact of such a transition on safety, comfort, and parking is examined, and policies that might be adopted by the Federal Government to encourage such a transition are investigated.

How Small Is Practicable?

The first question is, in essence: How small can a private car be and yet satisfy safety, emission, comfort, cost, aesthetics, and performance criteria acceptable to the consumer and to current/proposed government regulation. Our findings suggest that a private passenger automobile with a curb weight somewhat below 1500 lb can be built and that it would be acceptable in today's market with respect to performance and comfort. Currently the lightest automobile sold in this country is the Honda Civic which has a curb weight of 1700 lb. A reduction in weight to less than 1500 lb implies a small, two-passenger, limited-performance vehicle for urban use. The major problem is safety, and it is concluded that an increase in fatalities or serious injuries resulting from a major shift to small cars may be on the order of 15% unless some measures are taken such as a reduction (and enforcement) of speed limits, improvement and more extensive use of passenger restraint systems, and improved structural design.

Future emission goals also represent an unknown as they act counter to the requirements on fuel conservation and cost. In this area, it is suggested that the current California standards be adopted as the Federal standards and that a further

reduction not be considered for a period of 5 years. There do not appear to be any technological reasons why a small, clean, economical, and safe private automobile, with a curb weight less than 1500 lb, cannot be mass produced.

Effecting a Transition to Small Cars

Current automotive industry marketing is directed toward making the consumer aware of fuel economy as evidenced in recent advertisements. The methods considered in this report are those that can be formulated into legislation by the Federal Government with an attempt to compile what is known regarding price elasticities (i.e., a measure of the effect of a price change on the demand for a product). A review of the current literature has shown that the pertinent long-run elasticities vary over a considerable range so that the long-run market response to increased costs due to taxes and/or rebates cannot be predicted with great certainty. It is felt, nevertheless, that a shift to small cars, through government policy, might best be effected in the short run by tax/rebate policies designed to raise exponentially the original investment cost of automobiles as their fuel economy declines, and that large increases in the cost of gasoline must occur to effect a significant reduction in gasoline consumption.

Transportation and Economic Effects

The conversion to small cars will have significant effects on transportation and the economy. The effects on transportation can be great if the majority of cars are small. Traffic conditions would be improved and a large portion of the parking problems would be alleviated, assuming the number of vehicles does not increase 2 or 3 fold.

The effects on the economy are difficult to assess, and a meaningful analysis would require better data than currently available. A "first approximation" analysis of the industries that supply the raw materials necessary to manufacture the automobile indicates that the effects could be large, e.g., an 8% reduction in sales for the steel industry. A previous study (Ref. 1) has attempted to correlate the automobile weight to the employment in the auto manufacturing industry and concluded "that 1 percent change in new car weight results in a greater than 1 percent change in auto manufacturing employment."

It has been concluded that the effects on the economy will be large, and it is recommended that a detailed study be initiated using economic methods such as input-output analysis in order to account for the interrelationship of the various economic sectors.

An APL report is being published to detail and document the results.

Principal Investigators: L. L. Perini and R. A. Makofski. Mr. Perini is a senior engineer of the Aeronautics Division and Mr. Makofski is Supervisor of the Transportation Technology Group of the Aeronautics Division.

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WATERJET ACOUSTICS

A limited number of tests were conducted to determine the underwater radiated noise level resulting from a waterjet stream impacting a water surface. The data and theoretical considerations indicate that the acoustic intensity increases approximately as the first power of the flow rate. The efficiency of energy transfer is of the order of 10^{-8}.

The Surface Effect Ship (SES), the Surface Effect Vehicle (SEV), and the hydrofoil are all marine vehicles currently in development by the United States Navy. Concurrent with the crafts development, applications engineering and supporting effectiveness studies are being performed. Among other considerations the high speed of these advanced surface craft make them desirable candidates for ASW missions. The potential for ASW necessitates an understanding of the detailed acoustic emission of the craft, with particular emphasis on the slow-speed operating region appropriate to deploying ASW sensor systems.

The propulsion systems considered for these craft are air propeller, supercavitating, fully submerged or partially submerged, and waterjet. In the case of the waterjet, little or no empirical or theoretical data were available to permit a comparison to be made with other forms of propulsion or to determine how emitted noise varies with parameters such as ship size and speed. To gain some insight into these parameters a brief theoretical and experimental investigation was undertaken.

Two types of experiments were conducted to determine the underwater radiated noise from a waterjet. In the small-scale test a stream of water from a hose with a 3/4-inch nozzle was positioned over a tank filled with water. In the large-scale test water was pumped through a fire hose (1¼-inch nozzle) into a water-filled quarry. Hydrophones and test instrumentation completed the test setup to record the acoustic intensity. The primary test variables were water pressure and the height of the nozzle.

The data from the fire-hose test were processed on the CSS-3 real time analyzer using a processing bandwidth of 200 Hz. Two typical spectra are shown in Fig. 1. Broadband intensity was determined by integrating from 200 Hz to 20 kHz.

Theoretical considerations, based on the geometry and energy of the impacting jet stream, indicated that the noise level (dB) could vary as 10 log R, where R is the flow rate

(ft^3/s), which is equivalent to a variation according to 5 log P, where P is the dynamic pressure. As shown in Fig. 2, a noise increase according to 5 log P fits the data quite well. The variation of the noise level with the nozzle height, h, was generally within the accuracy of the experiment. Comparison with published data on rainfall (Ref. 1) showed a reasonably good correlation, the increase in acoustic level with computed dynamic pressure being nearly the same.

The efficiency, η, of energy transfer, expressed as the rate of the acoustic power output to the waterjet power, is

$$\eta = \frac{2 P_a a^2}{\rho R^3} ,$$

where

P_a = acoustic power output,

R = flow rate,

ρ = water density, and

a = cross sectional area of the nozzle.

The efficiency, based on the data and the above equation, is of the order of 10^{-8}

Principal Investigators: C. R. Brown and T. R. Small. Mr. Brown is senior mathematician and Mr. Small is senior engineer of the Fluid Mechanics Group of the Aeronautics Division.

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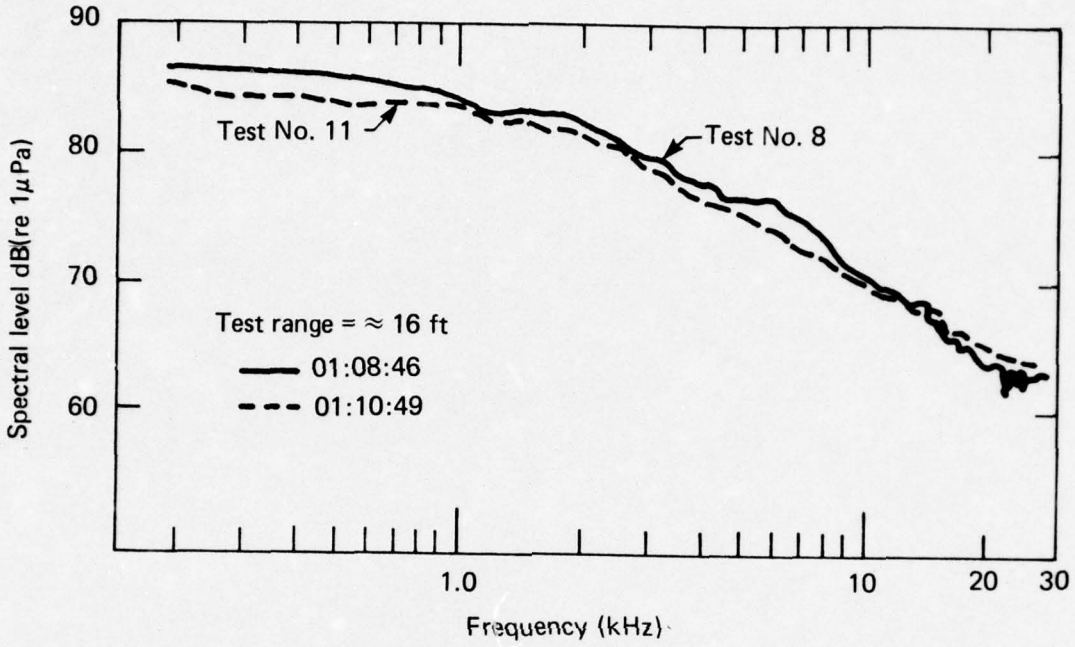

Fig. 1 Waterjet Spectrum

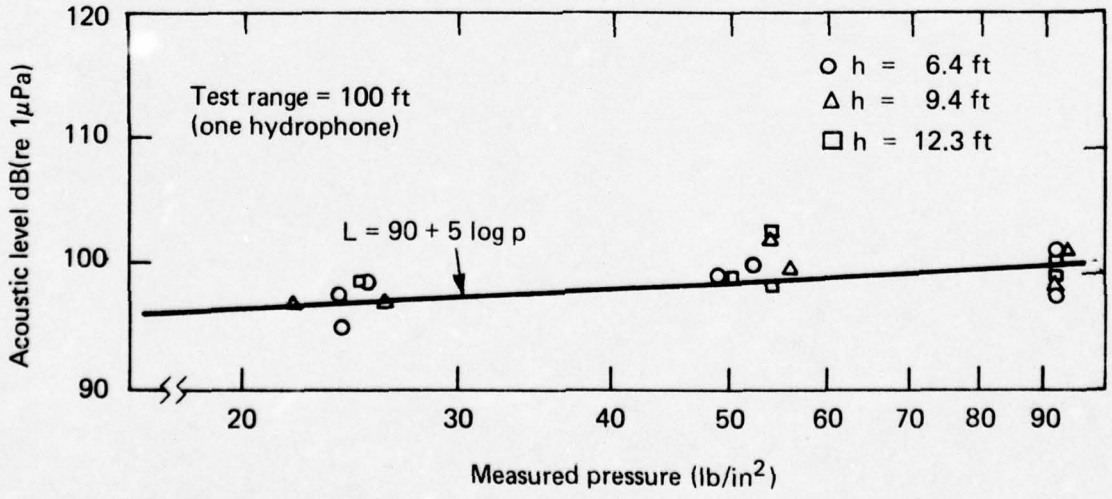

Fig. 2 Waterjet Test Results, 200 Hz – 20 kHz

MINI-RECORD DATA RETRIEVAL SYSTEM

Rapid access to medical records poses numerous problems that can be alleviated by computers. APL, with its broad experience in computer technology and its association with the Johns Hopkins Medical Institutions, is in an advantageous position to contribute to the solution of such problems. In the present project, a data retrieval system has been developed that is suitable for clinics such as the General Medical Clinic of the Johns Hopkins Hospital. The system was placed in operation and released to the Hospital for use and evaluation at their expense.

The Mini-Record Data Retrieval System is a new exploratory IR&D project that was both initiated and completed during the present reporting period. The primary objective was the development and demonstration of the use of a low-cost, medical-summary/problem-list retrieval system for General Medical Clinic outpatients. The development was carried out in collaboration with the staff of the Johns Hopkins Hospital, which is now supporting an extensive evaluation of the system.

The Mini-Record Demonstration was designed as a health care delivery aid that would:

1. Provide minimal information so that a patient is not placed at undue risk either from unnecessary diagnostic procedures or from inappropriate new prescriptions during an unscheduled encounter;

2. Provide continuity of medical care for those patients who rely upon the General Medical Clinic as their primary source of health care or are currently being treated by more than one clinic. This should result in better follow-up of known problems;

3. Facilitate the implementation and use of telephone inquiry service for General Medical Clinic patients; and

4. Assure the presence of an easily maintained patient medical-summary/problem-list in the Medical Records of all General Medical Clinic patients.

The Johns Hopkins Hospital performs the services of family physician for the local population as well as for a fairly extensive outpatient referral from the suburban hospitals. The General Medical Clinic is that clinic that accepts the ongoing

care of outpatients with chronic problems that do not fall within the specialty clinics, e.g., diabetes. However, General Medical Clinic patients do visit specialty clinics or the Emergency Room.

The General Medical Clinic treats approximately 7000 patients a year. It was selected for this pilot effort because of the potential advantages of an on-line Mini-Record system for a group of this size and varied makeup.

The APL-supported part of the project was performed in three phases: Requirements Definition, Program and Data Base Development, and Operational Demonstration over a period of five months. At the end of this period the fully operational system and data base was transferred to the Johns Hopkins Hospital for operational use and an extended evaluation.

Requirement Definition. Specifications were established for the demonstration system. Each General Medical Clinic patient visiting the clinic has a Mini Record that contains (a) demographic and administrative information, (b) brief text descriptions of major medical problems and/or history, (c) identification of medications currently prescribed, and (d) an indication of visits to other outpatient clinics since the last General Medical Clinic encounter. The Mini Record is available for display from interactive terminals; a hard copy of the most recent Mini Record is maintained in each patient's medical folder. Access to the on-line Mini Record is by either patient history number or name from any of three clinics. Finally, procedures were set up to maintain the data base, automatically capture data, and manage processing flow.

The Program and Data Base Development. Information for the data base was obtained from (a) an Encounter Form, which was filled out for each General Medical Clinic visit, (b) the billing file, which recorded all visits to other clinics, (c) discharge summaries, which provided problem lists and medications for newly discharged patients scheduled for follow-up at the General Medical Clinic, and (d) physician-submitted corrections and additions to existing Mini Records.

Computer programs were developed to capture and process the data, display Mini Records interactively, print Mini Records and status reports, provide on-line and batch mode editing, and perform general support functions. In all, five major programs comprising over 3000 instructions were developed. All programs were written in PL/I for the IBM 360/91 for tests at APL.

Operational Demonstration was begun at the Hospital within three months after the beginning of the initial phase. The initial capability provided on-line access to a data base of approximately 2000 Mini Records. During the first month the Operational Demonstration was used for (a) general indoctrination, and (b) system refinement. As a result of experience with the on-line demonstration, operating procedures were modified and computer programs altered and expanded. By the end of the Operational Demonstration phase, all computer programs were fully tested, operational procedures were implemented with trained personnel, computer programs were transferred to execute on the Johns Hopkins Hospital computer, and a data base of over 5000 Mini Records was made available.

Evaluation

A preliminary evaluation was performed during the Operational Demonstration. It was decided that (a) all preliminary indications suggested that the system was an effective aid to the operation of the General Medical Clinic, (b) the Mini-Record system was a necessary prerequisite to establishing a desired telephone inquiry service for General Medical Clinic patients, and (c) an extended evaluation period would be required in order to assess the impact of the Mini Record and the telephone inquiry service upon health care delivery. As a result of the preliminary evaluation, JHH provided funds to operate the system after the APL funded demonstration period.

In brief, the system appears to be successful. Physicians are using the Mini Records, procedures for file update and maintenance are running smoothly, and all computer programs are performing correctly.

In addition to satisfying its stated objectives, the Mini Record Demonstration System produced ancillary benefits:

1. A request from the Office of Health Care Programs to assist in the evaluation of outpatient visit patterns and distribution;

2. Support to adapt and expand the system for Cancer Center Tumor Registry; and

3. The possible adaptation of the system (or its logic) for use in an on-line visitor control system for APL.

Principal Investigator: P. G. Casner. Mr. Casner is Group Supervisor of the Information Processing and Display Group of the Fleet Systems Department.

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